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THE INSTITUTE OF PETROLEUM

An Ordinary General Meeting of the Institute was held at 26 Portland Place, London, W.1, on 7 November 1956, the Chair being taken by W. H. Thomas, a member of Council.

The Editor read the minutes of the previous meeting, which were confirmed and signed as a correct record. He also announced the names of members elected since the previous meeting.

The Chairman, introducing the authors of the papers to be presented, said: There is a fast-growing interest in digital computers in the U.K., although in the U.S.A. they are in far more active operation, over a far wider area, than they are here. Therefore, it was thought opportune for the Institute to consider these matters.

Naturally, one is very interested in the various features and abilities of these machines and the tremendous saving in calculation time effected by their use.

The first paper is by J. H. Wilkinson, who is a senior principal scientific officer at the NPL, where he has been associated with the design of the pilot ACE computer and has indeed assisted in its construction. Since its completion he has been in charge of the group at NPL concerned with exploiting the pilot ACE and, more recently, the DEUCE machine. He will be dealing with the computer facilities which are available in this country. The paper provides an excellent background from which to consider the other three papers, which are concerned with the application of computers to various operations in the petroleum industry.

The second paper, on fundamental research, will be presented by Dr Barnett, who took his Ph.D. degree in the field of quantum mechanics at King's College under Professor Coulson. Following the Shelter Island conference on quantum mechanical methods and theory, Dr Barnett became involved with computing, using conventional punch card equipment for quantum chemical problems. He has been associated with the British Rayon Research Association and the Radar Research Fellowship, and has now joined IBM (United Kingdom) Ltd., having built up a group concerned with the scientific applications of his company's machines.

The author of the third paper, Dr J. T. Ahlin, is a graduate of the Californian Institute of Technology and was Professor of Mathematics at the University of Southern California. He joined the IBM Corporation in 1952, and is the applied science representative in the special petroleum department of his company at Houston, Texas, being responsible for relationships with users of computers in the petroleum industry throughout the U.S.A.

The final paper, by B. D. Dagnall and P. Mayers, of the Esso Petroleum Company, deals with the application of the instruments to one or two specific refinery problems. Unfortunately Mr Dagnall is in the U.S.A., but Mr Mayers will present this paper. Mr Mayers graduated from the chemical engineering department of the University of Birmingham in 1951 and joined Esso in 1953 as a process engineer. He was responsible for the technical aspects of catalytic cracking, and after a visit to the U.S.A. and the installation of a computer at Fawley he has been responsible for the computer programme of catalytic cracking correlations.

SYMPOSIUM ON DIGITAL COMPUTERS IN THE PETROLEUM INDUSTRY

COMPUTING FACILITIES IN GREAT BRITAIN*

By J. H. WILKINSON

INTRODUCTION

ALTHOUGH the idea of constructing a computer which would carry out automatically-extended sequences of arithmetic operations is more than a hundred years old, it was not until the development of modern electronic pulse techniques during the second world war that the project began to achieve its present-day significance. It is with the developments which have taken place since the advent of these techniques that this paper is concerned.

The first truly electronic computer was constructed during the war by the Moore School of Electrical Engineering, University of Pennsylvania. This machine, ENIAC (Electronic Numerical Integrater and Computer), was built specifically for the calculation of ballistic tables, but it proved sufficiently flexible to be used as a general purpose computer. Its main component parts were 20 electronic storage registers, each capable of storing one ten-digit decimal number and of adding to it (or subtracting from it) a number transmitted from any other register, a set of switches on which 300 numbers could be set up by hand, and an arithmetic unit capable

* MS received 7 October 1956. Communication from National Physical Laboratory, Teddington.

of performing multiplication and division and of taking square roots. To prepare the machine for solving any problem, it was first necessary to reduce that problem to a series of arithmetic operations. The units of the machine had then to be interconnected by means of an extensive system of plugs and sockets, the particular nature of the interconnexions determining the sequence of operations which the machine would carry out. This was a tedious and lengthy operation and, moreover, it had the disadvantage that if further runs on a problem were needed after the set-up had been changed, the whole process had to be carried out again.

In spite of its limitations the successful completion of ENIAC in 1946 was a remarkable achievement, and although it contained some 18,000 valves and 1500 relays, it worked remarkably well. The speed of computation was of a different order from that achieved before; some measure of the speed may be assessed from the fact that it took 200 microseconds to add two numbers together and 2·8 milliseconds for their multiplication.

THE MODERN HIGH-SPEED COMPUTER

After the completion of ENIAC, work was started almost simultaneously in a number of research establishments here and in the U.S.A. on the construction of automatic electronic computers. Although these machines differed substantially in detail, they were basically much the same. They differed from ENIAC in that the number of storage registers was increased by a factor varying from 10 to 50, and also in the way in which they were prepared for the solution of a problem.

The first change was achieved by abandoning the direct use of valves as storage units and using instead a number of physical devices such as mercury delay lines and cathode-ray storage tubes, which were much more economical.

The second change was even more fundamental. The arithmetic operations involved in a computation were stored in coded numerical form in the same storage registers as were cased to hold the numbers. The way in which this was achieved may be described, quite simply, as follows. Suppose the machine has a thousand registers, and these are numbered consecutively from 000 to 999. Then a typical arithmetic operation, *e.g.* an addition, could be described as follows.

"Take the number in register 329 and add it to the number in register 50 and send the result to register 360."

This could be written symbolically.

$$329 + 050 \longrightarrow 360$$

If one restricts oneself to the four arithmetic operations addition, subtraction, multiplication, and division and these are numbered 0, 1, 2, and 3 respectively, the above operation may be written

329, 0, 050, 360

or, if the commas are omitted, as a ten-digit number. Such a "coded construction" may therefore be stored in one of the machine's registers exactly as though it were a number.

In addition to the storage units and the arithmetic facilities the machines contained a control unit, which interpreted the stored instructions and supervised their execution, and an input–output unit by means of which the data and the coded instructions were introduced into the machine and the final answers were communicated from it. On most machines the input unit consisted of a punched card or punched tape reader, and the output unit of a card punch, tape perforator, or typewriter.

To prepare a problem for these new machines it has first to be reduced to a series of arithmetic operations just as for ENIAC; a set of coded instructions must be prepared describing these arithmetic operations, and these instructions must then be punched on the input medium together with the input data. The process of preparing the coded instructions is usually called programming, and the development of satisfactory programming techniques has been one of the major tasks associated with using the new machines. Once a programme has been prepared for the solution of a particular problem, specific "runs" on that problem may be performed very quickly. Thus, having prepared a programme for the inversion of matrices, any matrix may be inverted using this programme, provided it does not exceed the storage capacity of the machine. All that is needed is that the matrix data should be punched on the input medium and that this data, together with the programme, should be read into the machine. There is no further programming to do on that particular problem. Similarly, to take a computation in an entirely different field, once the programme for calculating a pay-roll has been produced this same programme may be used indefinitely or until there is some fairly fundamental change in the method of accounting used. Because of this the intellectual capital which is invested in the production of a specific programme continues to yield dividends throughout the life of the machine for which it was devised.

Although in many respects the construction of ENIAC's successors appeared to be a somewhat simpler task than building ENIAC itself, this did not in practice prove to be true, and the time taken to complete successful working models was somewhat longer than most of the workers in this field had expected. The first machine to demonstrate successfully the new principles was built at Manchester University. This was not a very ambitious project, and was never really used for serious computation,

but its completion in 1948 was a landmark in the history of computers. It was followed in 1949 by EDSAC at Cambridge University, and much of the pioneering work in connexion with the use of computers was done on that machine. The techniques developed at Cambridge have formed the basis of the system used on many computers throughout the world. Probably the first two computers to be used on a production basis were SEAC, at the National Bureau of Standards, Washington, and Pilot ACE at the National Physical Laboratory, Teddington; both of these machines came into operation during 1950.

It might well be said that with the completion of these machines the success of the new computers was assured, but it was soon obvious that their full impact would not be felt until machines of a high standard of reliability were readily obtainable commercially. Although one of the earliest machines, the Ferranti Mark I, was produced in this country, it has taken longer than one might have hoped for machines to be produced in satisfactory numbers, and it is only comparatively recently that the purchaser of an electronic computer has been provided with a choice of machine. Even at the present time, however, the delivery dates of machines on the market in this country are far from satisfactory. In the U.S.A., on the other hand, commercial production has advanced much more rapidly, and there is a very considerable number of machines already in operation, both in the scientific and commercial fields of application.

The remainder of this paper is concerned with a brief account of the main features of high-speed electronic computers and concludes with a classification of a number of available machines.

COMPUTER CHARACTERISTICS

Probably the simplest way to deal with the machines which are available would be for the author to give a frank assessment of the merits of each, while trying to achieve a strict impartiality. Unfortunately, this is unpractical because it would be too lengthy, and impolitic for the following reasons. Most machines represent a compromise between what is desirable on the one hand and what can be provided with available resources and at a reasonable cost on the other. Because of this they all have shortcomings of which the designers are usually quite well aware, but which the manufacturers are naturally reluctant to admit. Accordingly, there is a brief account of the more important characteristics of a computer and this is followed by a classification of a number of existing machines.

(1) *Number System*

Most desk computers (except those designed specially to deal with sterling) use a decimal representation of numbers. On high-speed computers this form of representation is comparatively uncommon, and a binary (or scale of two) representation is usually preferred. In the decimal scale each number is represented by the sum of multiples of powers of 10.

Thus

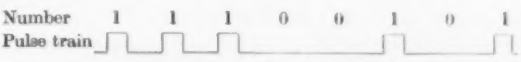
$$9653 = 9 \times 10^3 + 6 \times 10^2 + 5 \times 10^1 + 3 \times 10^0$$

Similarly, in the scale of 2 each number is represented as the sum of multiples of power of 2, and just as in the decimal scale the multiples are all less than 10, so in the binary scale all multiples are less than 2, and the only digits are therefore 0 and 1.

Thus

$$10111 = 1 \times 2^4 + 0 \times 2^3 + 1 \times 2^2 + 1 \times 2^1 + 1 \times 2^0$$

and is the binary equivalent of the number 23. The reason for this preference is that, in the scale of two, arithmetic operations are particularly simple and, moreover, binary numbers admit of a simple representation electronically. Two main classes of computer are recognized, known respectively as serial and parallel. In a serial machine a number is represented by a train of pulses which travel on a single channel. The pulse representation of a number is shown below.



In parallel machines there are as many channels as there are digital positions in a standard number. All the digits are transferred simultaneously, each on its own channel. Other things being equal, a machine which works in the parallel mode is faster than a machine working in the serial mode. The programme, however, is not directly concerned with this aspect of the machine. There are some machines in which a decimal representation of numbers is used internally, but even in these each decimal digit is usually represented separately in binary form (often called binary decimal representation). The following is an example of such a representation:

$$975 = 1001, 0111, 0101$$

On all binary machines initial data are inserted, and final results expressed, in decimal form, the conversion from decimal to binary during input, and from binary to decimal during output, being achieved by a set of instructions. In the author's experience the internal use of binary is of negligible inconvenience, but he is almost persuaded that for commercial arithmetic the complications introduced in the construction of the machine by using a decimal representation are justified.

The length of number used is usually from 30 to 40 binary digits, which is equivalent to 9 to 12 decimal

digits. The term "word" is used for such an aggregate of digits. This is to cater for the fact that it may represent a number or an instruction.

To the practical physicist or engineer the number of digits in a word may appear to be unnecessarily large, but it should be remembered that extra digits are necessary in long calculations to guard against the accumulation of rounding errors, and nominal accuracy must not be confused with the final accuracy of results used for practical purposes.

In all the early machines a "fixed" binary point system was used so that numbers, x, were regarded as lying in some prescribed range, usually

$$-2 \leq x < 2$$

In order to keep numbers within range it was necessary to introduce scale factors. For some problems the analysis needed to provide appropriate scaling was the most difficult task involved in preparing the programme. For problems in which this proved prohibitively difficult a different system of representation was adopted. Each number, x, was represented in the machine by a pair of numbers a and b, chosen so that

$$x = 2^a \times b$$

where a is an integer positive or negative, and b satisfies.

$$\tfrac{1}{2} \leq |b| < 1$$

This is usually called a "floating" system of representation.

When this scheme was adopted a programme consisting of a number of instructions (usually called a "subroutine") was necessary for each of the fundamental arithmetic operations. In some of the more advanced machines the computer itself operates normally on numbers in floating form so that the need for a whole programme of instructions in order to execute a single arithmetic operation is avoided.

(2) *Storage Registers*

In an ideal machine the number of storage units would be in excess of the number which would be likely to be required in any contemplated calculation. The registers would all be of one type and numbered consecutively, and would be such that numbers could be extracted from them or inserted in them in times which were small compared with the time of a multiplication. Unfortunately storage registers of this type are expensive, and even in the fastest British machines the number of registers of this type has been restricted. This is perhaps not true in the most advanced American machines, but these are very expensive.

In the faster British machines the store is usually divided into a "high-speed" section with from 200 to 1000 registers and a "backing-up" or "intermediate" store of much higher capacity. The high-speed store is used to hold those numbers and instructions in current use, and is replenished from time to time from the backing-up store.

The main high-speed storage devices in order of historical development are the following.

(a) *Mercury Delay Lines.* In this store numbers are remembered as sound waves in a column of mercury. The electrical pulses representing the numbers are applied to a piezo-electric crystal and the resulting vibration of the crystal is transmitted as a sound wave along the column of mercury and impinges on a crystal at the other end of the column. This produces a voltage pulse which is amplified and fed back again to the input crystal. In this way the pulse trains are remembered indefinitely. The main weakness of the store is that in order to economize on equipment, it is necessary to use units which hold quite a number of words. The average access time of a given word is half the circulation period and is consequently longer than one might expect for a given pulse repetition rate. Usually delay line machines contain a few stores holding one word each, in addition to those which hold the great bulk of the words.

(b) *Nickel Delay Lines.* These are very similar to mercury delay lines, the magnetostrictive properties of nickel wire being used to excite and detect the waves. They have the same "access time" weakness as mercury delay lines, and so far it has not proved possible to use such high pulse repetition rates. They are, however, much lighter and more compact. Both forms of store are most naturally used in the serial mode.

(c) *Electrostatic store.* The version of this store which has been used in this country is that due to Williams and Kilburn. The binary digits are stored as small charges on the surface of a cathode-ray tube, the charge distribution for a zero being different from that for a one. The charges slowly leak away, and before degeneration is too severe the tube is rescanned, the zero and ones detected and rewritten. This rescanning takes place at regular intervals. The only British commercial machine using this type of store works in the serial mode, but in the U.S.A. it has been extensively used in parallel machines.

(d) *Ferrite core store.* In this store individual binary digits are stored on very small ferrite cores. A core is said to be storing a one when it is magnetized in one direction and a zero when magnetized in the other. A complete store consists of a matrix of cores each being threaded by wires by means of which digits 0 or 1 may be written on, and subsequently read from it. Machines with very large stores of this type are already in

operation in the U.S.A., and at least two machines with moderate size stores are under construction in Britain.

(3) *Intermediate Stores*

Easily the most common form of intermediate store is the magnetic drum. Binary digits are stored as small dipoles in magnetic material which forms the coating of a rotating metal drum. Information is stored on a number of tracks round the drum, and each track is associated with a writing head and a reading head by means of which numbers may be written on, or read from it. Quite large stores are provided comparatively cheaply in this way. In the medium-speed machines the drum store is virtually the only store apart from a few arithmetic registers, but in most of the faster machines information is transferred from the drum to the high-speed store (and vice-versa) in blocks of 8 to 32 words at a time. Sometimes there are facilities for transferring, in addition, individual words. In many problems the drum store is fully equal to the same amount of high-speed store. These problems are characterized by the fact that the time taken to transfer a block to the high-speed store is small compared with the time taken to use that block. In other problems where a random or unsystematic reference must be made to information on the drum, the access time results in a great loss of speed. Even when the high-speed store is well integrated with the drum store, the combination is never quite as convenient as would be a single large high-speed store.

A second form of intermediate store is provided by magnetic tape. Numbers are stored as dipoles in magnetic material which has been sprayed either on paper or on cellulose acetate. Magnetic tapes can provide almost unlimited storage, but the access time to an arbitrary word on the tape is correspondingly high. Tapes are seldom used as alternative to drums, and in general serve a very different purpose. They are of great value for problems involving large volumes of data, as is common in commercial computation. The development of tape systems has received somewhat less attention here than most other aspects of high-speed computing, and although they will be added to most machines in due course, few if any commercially-produced machines have yet been delivered with a fully operative tape system.

Checking Digits. It is possible to provide a check on the performance of any form of store by including redundant information. The principle is the same for all stores, and will be described in connexion with magnetic tapes on which it is most commonly used. Information on a magnetic tape is usually provided on a number of channels, six channels being fairly common. A seventh channel may be included on which a 0 or 1 is recorded, so chosen as to give an odd total of ones. A similar check digit may be used on each word stored in any of the high-speed stores or on a magnetic drum.

(4) *Order Code*

The simplest classification of order codes is by the number of storage registers specified in an instruction. In the example given above, three storage registers (or "addresses") were mentioned, and such a code is usually called a three-address code. The most common type of code is that in which one address only is mentioned and one arithmetic or similar operation. All operations are associated with a single central register usually called the accumulator, so that this is not explicitly referred to in the instruction. Typical operations are the following

$$+_c 57$$

meaning, "clear the accumulator and add the number in register 57 to it,"

or $+57$

meaning, "add the number in register 57 to the accumulator without clearing it previously,"

or $T57$

meaning, "transfer the number in the accumulator to register 57." To achieve the three-address operation

$$A + B\,C,$$

three one-address operations are required

$$\begin{array}{l} +_c A \\ +\ B \\ T\ C \end{array}$$

but this gives a very one-sided impression of the relative effectiveness of the codes, for two reasons. First, one-address instructions are usually sufficiently short for two to be stored in each word, and secondly, when a sequence of operations is required, the ratio of the number of one-address to three-address instructions is decreased. This would happen, for example, if five numbers were added together instead of two.

In many machines consecutive instructions to be obeyed occupy consecutive storage locations, and this is obviously the most natural course to adopt. Where the high-speed store is of the type for which access time tends to limit the speed of operation, this shortcoming can be overcome in some measure by placing instructions in such relative positions in the store that the next instruction usually becomes available just as the previous one is completed. Since for such codes the position of the next instruction is not determined by a fixed rule, each instruction contains an extra address specifying the position of the next instruction. It is customary to regard this last address as different from the others and to refer to $3 + 1$ or $1 + 1$ address codes as the case may be.

TABLE I

Computer Characteristics

Computer	Number case	Word length	Order code	High-speed store	Intermediate or main store	Mode of operation	Times for arithmetic operations		Input medium and speed	Output medium and speed	Approx cost
							Floating	Non-floating			
Edsac I	Binary	34 binary	1 address	Mercury delay lines, 512 words	Magnetic tapes	Serial	—	Add 1½ millisec. Multiply 4 millisec	Punched paper tape, magnetic tape	Punched paper tape, typewriter magnetic tape	—
Ferranti Mark I	Binary	40 binary	1 address	Williams and Kilburn, 256 words	1 Magnetic drum, 16,384 words	Serial	—	Add 1 millisec. Multiply 2 millisec	Paper tape, 200 characters/sec	Pinched paper tape, teleprinter	£80,000
Deuce	Binary	32 binary	2 + 1 address	Mercury delay lines, 400 words	1 Magnetic drum, 8192 words	Serial	—	Add 64 μsec. (min *) Multiply 2 millisec Divide 2 millisec	Punched cards, 200 words/min equiv to 6000 decimal digits	Punched cards, 100 cards/min equiv to 3000 decimal digits	£42,000
Pegasus	Binary	39 binary	1 address but with 7 accums.	Nickel delay lines, 55 words	1 Magnetic drum, 4096 words	Serial	—	Add 300 μsec Multiply 2 millisec Divide 5·5 millisec	Paper tape, 200 characters/sec	Punched paper tape, teleprinter	£43,500
Elliott 402	Binary	32 binary	1 + 1 address	Nickel delay lines, 15 words	1 Magnetic drum, 2944 words	Serial	—	Add 200 μsec * (min) Multiply 3·2 millisec Divide 3·2 millisec	Paper tape	Paper tape and on teleprinter	£28,000
Mercury	Binary	40 binary	1 address	Magnetic cores 256–1024 words (varies with price)	4 Magnetic drums, 4096 words each; 8 may be fitted	Serial arithmetic operations	Add 180 μsec Multiply 300 μsec	Mainly floating counting, etc, non-floating 60 μsec	Paper tape, 400 characters/sec	Paper tape, 33 characters/sec	£90,000 for full store
Edsac II	Binary	40 binary	1 address	Magnetic cores 1025 words + extra	Magnetic tapes in first instance	Parallel	Add 75 μsec (av) Multiply 275 μsec Divide 250 μsec	Add 20 μsec Multiply 200 μsec Divide 200 μsec	Paper tape	Paper tape	—
Ace (full scale)	Binary	48 binary	3 + 1 address	Mercury delay lines, 800 words	Magnetic drums (4), 8192 words each	Serial	—	Add 32 μsec * (min) Multiply 400 μsec Divide 1·5 millisec	Punched cards, 400 words/min equal to 32,000 decimal digits	Punched cards, 100 words/min equal to 8000 decimal digits	—
Decca C1	Decimal insts. in binary	10 dec. 40 binary	1 + 1 address	Magnetic register 16 words	1 Magnetic drum, 4032 words	Serial	—	Add 470 μsec * (min) Multiply 10 millisec (av)	Paper tape, 200 characters/sec	Type-writer, 16 characters/sec Teleprinter, 7 characters/sec	£19,000

* Optimum coding.

In the same way loss of speed due to access time may be cut down by the appropriate spacing of numbers as well, or instead of, instructions. Machines in which any or all of these devices are employed are said to use "Optimum Coding." Altogether the advisability of using optimum coding is a very vexed subject. At the risk of being dogmatic, the author would say that optimum coding with respect to instructions is of great value and requires little extra programming effort, provided the machine is well designed with this in mind. Optimum coding with respect to numbers is, however, usually unsatisfactory, and with respect to both numbers and instructions simultaneously is a practical impossibility.

It is, of course, possible to use a machine designed for optimum coding and place instructions in consecutive positions. In this case one still has the benefit of the optimum coding in the subroutines.

As regards the operations provided, all machines so far built for serious computation have included addition, subtraction, and multiplication. Division, on the other hand, has sometimes been included and sometimes not. In the early machines the omission of a division order seemed a reasonable economy, since a division can be effected when necessary by a small subroutine using multiplications. However, in the opinion of the author, the case of including it in machines which are being constructed now is very strong. Instructions for shifting numbers to the left and right by an arbitrary number of positions are important, as also are the instructions used for making decisions during the course of a programme. In addition to arithmetic operations, order codes usually contain instructions which perform logical operations on pairs of numbers. It is a mistake to dismiss these as frills which are added for the benefit of mathematicians. They are very useful in many computations of a practical nature.

(5) *Library of Programmes and Subroutines*

When the first machine of a given type is produced a good deal of work has to be done before it can be used effectively. Subroutines must be produced for all the elementary operations such as decimal–binary and binary–decimal conversion, extraction of square roots, evaluation of sines, cosines, exponentials, logarithms, and many others. Later programmes are produced which deal with many of the standard problems of numerical analysis such as solving differential equations, finding zeros of polynomials, solving linear algebraic equations, or inverting matrices. The nature and extent of the existing library of subroutines card of programmes is of great importance to any purchaser of a machine, particularly if the machine is to be used by a fairly small group for which the production of its own library would be a formidable undertaking.

(6) *Input and Output*

Two main forms of input and output have so far predominated, paper tape and punched card. Where punched tape is used as the output medium printing is usually provided by a teleprinter. Results are frequently obtained both on tape and in printed form. Where cards are used for output, printing is usually performed away from the machine on a tabulator or less frequently on a card-operated typewriter. In the U.S.A. a number of machines may print out results at high speed using a line printer. Only one British machine, the Ferranti Mark I, has had an output of this type. This was provided by a Bull printer.

The main advantages of paper tape over cards are its low cost and compactness. Cards, on the other hand, have the advantage that individual numbers may be inserted, extracted, or replaced and it is particularly easy to locate and identify a specific item in a group. On the whole there is a distinct tendency on the part of users to prefer the medium of which they have had more experience (often their only experience), but, as a card enthusiast, the author would like to mention that more than one group has changed from tape to cards, but he knows of no change that has taken place in the reverse direction!

AVAILABLE COMPUTING FACILITIES

The accompanying table displays the main characteristics of a number of available computers, including both commercial and non-commercial machines. No attempt has been made to give an exhaustive table, but a fairly wide range is covered. One has only to attempt to produce such a table to realize how controversial even the simplest entry may become.

For example, the speed of the arithmetic operations would appear to be quite a definite concept, but quoted figures may include or exclude the time taken to extract the instruction and/or the access time of the operation.

In addition to selling computers, several firms now provide a computing service and using this service is a useful way of finding out about computers and what is involved in solving problems on them. One of the most interesting developments in the computer field has been the formation of a special panel by the Society of British Aircraft Constructors to co-ordinate and rationalize the problems that arise in the aircraft industry. Further experiments of this kind may make the greatest contribution to the practical application of modern high-speed computers.

ACKNOWLEDGMENT

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SOME APPLICATIONS OF ELECTRONIC DIGITAL COMPUTERS TO FUNDAMENTAL RESEARCH IN THE PETROLEUM INDUSTRY *

By M. P. BARNETT †

INTRODUCTION

A WIDE diversity of topics can be included under the heading of fundamental research, relevant to the petroleum industry. If fundamental research for the petroleum industry is to be defined, by a process of elimination, as that research which cannot readily be included under the headings of refinery control or process development, then the totality of hydrocarbon research, of laboratory work on fractionation processes, of vapour phase catalysis studies, to mention but a few subjects, become eligible immediately for inclusion. Developments in the petrochemical industry can well extend the reference to hydrocarbon research into a reference to the full range of aliphatic chemistry. Problems of petroleum prospecting bring into the picture theories of oilfield structure and reservoir behaviour, and even of oilfield genesis. Rather than attempt a comprehensive survey of computer applications in physical, physico-organic and analytical chemistry, chemical engineering, and geophysics that bear on petroleum and petroleum chemical work, a few representative topics will be discussed in turn.

ANALYTICAL TECHNIQUES

Certain experimental techniques provide a powerful means of chemical analysis marred only by the accompanying need for heavy computation. Mass spectrometry provides a very striking example. As a tool in analysing mixtures of gases that are chemically inert, particularly in petroleum work, the mass spectrometer has achieved great popularity over the last few years. As a result of extensive use in monitoring analyses for actual plant operation, mass spectrometric calculations could find a place under refinery control, but the use of mass spectrometric analysis in the research laboratory justifies this present mention of the subject.

In mass spectrometric analysis, a gas sample is ionized by bombardment with ions of controlled energy range, and the resulting cracked mixture separated into beams of different mass to charge ratios by a magnetic field. The ion currents corresponding to different beams are measured, so giving the different "peak heights" in terms of some arbitrary unit. These peak heights are simply the peak heights for the individual species present, weighted in proportion to their respective contributions to the mixture and combined additively. To calculate the proportions of components in the mixture, a set of simultaneous equations must be solved, in which the coefficients are terms of the cracking patterns for the individual hydrocarbons, and the right-hand sides are the sets of peak heights observed for individual analyses. For work in which the cracking pattern of the instrument remains constant for several months, the preparation and retention of the inverse matrix is feasible, and each analysis requires just the multiplication of this inverse matrix with the appropriate peak height vector. Quite small machines have been used for this work, *e.g.* the IBM 626 calculator, in which arithmetic is determined by the wiring on a control panel or plugboard.[1] Larger machines, *e.g.* IBM 650 [2] and Ferranti Mark I*, have been programmed to work from the actual equations. Some such programmes use more peak heights than there are components. This amounts to the inclusion of a certain amount of information that would be redundant, were the experiments and basic data completely accurate, but which under the actual working conditions permits a better estimate of the final results to be obtained, for example, by least squares methods.

ANALYSIS OF EXPERIMENTAL DATA

A further use of computers as an adjunct to laboratory experiments occurs in connexion with the manipulation of a set of results relating to the same quantity or quantities, to obtain the values which can be considered "best" in the statistical sense. One example is the mass spectrometric calculation mentioned at the end of the previous paragraph. Other examples relevant to petroleum work can be found amongst determinations of gas law constants (parameters in the equations that relate pressure, temperature, and volume) and in phase change relationships. In general, several sets of numbers are obtained, such that the individual sets when substituted in certain equations should cause these to balance numerically. The coefficients in the equations, however, are not known, initially, and in fact are the quantities to be derived from the experimental results. Substitution of the experimental data provides sets of equations for the unknowns which cannot all be solved exactly and simultaneously. Solutions are sought that minimize the sum of squares

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of the departures from balance of the equations into which individual sets of results have been substituted. Peculiar forms for the equations, *e.g.* when they contain logarithms,[3] may complicate the procedure for calculating the unknowns, *i.e.* the coefficients, but the calculation always entails in effect the solution of a set of simultaneous equations. This is a standard problem for the computer. Further examples can be found in the fitting of rate constants to kinetic data.[4]

EXPERIMENTAL INVESTIGATION OF MOLECULAR STRUCTURE

The computer, as an aid to the interpretation of experimental data, has found perhaps its longest and most extensive application in crystallographic work. Crystallographers did, in fact, seek aid from conventional punched card equipment in the pre-electronic computer age, and Fourier syntheses and least squares refinement procedures have been programmed for practically every type of high-speed machine now in existence.

The objective of any crystallographic investigation is the determination of the distance between the atoms in a molecule, or in adjacent molecules, in a regular crystalline substance. A beam of parallel X-rays, fired at a specimen of the material, is split, as a result of diffraction by the atoms, into a large number of emergent beams, the intensities of which are recorded by their blackening effect on a photographic plate. After some preliminary manipulation of the data, a reasonable gauge can usually be obtained from chemical considerations as to the approximate arrangement of the atoms in the unit cell. From the set of co-ordinates that approximate the atomic positions, it is possible to calculate certain quantities (the structure factors, denoted usually by F^{hkl}), which can also be derived from the data observed experimentally. The calculated values, F^{hkl}_{calc}, will differ in general from the values F^{hkl}_{obs} derived from experiment. The discrepancies, and certain quantities related to the F^{hkl}_{calc}, which are computed at the same time as the F^{hkl}_{calc}, may be used to calculate corrections to the values of the atomic co-ordinates which were assumed for the calculation of the F^{hkl}_{calc}. These improved atomic co-ordinates can then be used to recalculate fresh values of the F^{hkl}_{calc} which should agree more closely with the F^{hkl}_{obs}. Comparison of the new F^{hkl}_{obs} leads to further refinements to the co-ordinates of the atoms in the crystal. This process of calculating in alternation, increasingly refined values of the atomic co-ordinates, and of the calculated structure factors, can be continued until successive refinements cease to have any appreciable effect on the positions calculated for the atoms. The procedure as just described constitutes the "least squares" method for "refining," *i.e.* improving, the structures pictured for molecules. This least squares method has been programmed for a number of machines, including the IBM 704.[5] It can lead to very high accuracy in the final answers, but is obtained as a result of an appalling amount of computation. The time needed to complete a single iteration on the 704 is roughly $AR/20{,}000$ hours, where A is the number of atoms in the basic asymmetric unit of the crystal, and R is the number of reflections included in the calculation. Another approach to the refinement problem, and equivalent to the least squares method, is the method of differential synthesis, programmed, for example, for the Manchester University computer.[6] In this method there is again an alternation back and forth between quantities that are assumed, and quantities calculated from them for a comparison with experiment, that will provide further corrections to the assumed quantities.

THEORETICAL CALCULATIONS OF MOLECULAR STRUCTURE

The energies associated with particular molecules, or of fragments or aggregates of molecules, in different geometrical configurations or states of electronic excitation, are of very considerable interest. Indeed, these energies would, if known completely, provide the totality of thermodynamic and spectroscopic information about the systems concerned. The manner in which such energies, derived either from theory or experiment, are processed to yield thermodynamic data is described in the section which follows. Computers may in fact be used in this later stage of thermodynamic prediction. Although the energies can often be found from experiment, however, many advantages follow from an ability to derive them completely from theoretical considerations. For example, expensive and time-consuming organic separations or syntheses, followed by elaborate physicochemical measurements, might be avoided if the thermodynamic properties of new substances could be predicted in advance of their isolation. The ability to provide a complete and accurate theoretical prediction of the properties of, say, a 40-atom hydrocarbon, starting from a specification of just the rough structural formula, though possible in principle, cannot really be claimed as imminent by even the most enthusiastic advocates of the so-called "non-empirical quantum chemistry." The mathematical basis does in fact exist for effecting such predictions—the Schrodinger equation of wave mechanics yields the energy levels of a molecular system as the eigenvalues of a Sturm-Liouville type partial differential equation. This equation involves as independent variables, unfortunately, the space co-ordinates of all the electrons in the molecule. The direct solution of such an equation in just six variables (the hydrogen molecule) constituted an appalling problem for hand computation, even when

considerable analytical ingenuity had been used to reduce the numerical work by as much as was possible.[7] Wave mechanics has been applied extensively to molecular studies over the last thirty years, in two main ways. Many workers tried to find approximate solutions, within the framework of some standard procedures that were essentially mathematical in nature, but which had a certain chemical plausibility. This "non-empirical approach," as applied to relatively simple molecules, provided a number of interesting and significant qualitative results but, prior to the electronic computer decade, little in the way of dependable quantitative information. It gave rise to computations of two main types, first the calculation of certain quantities, termed molecular integrals, and secondly, the extraction of latent roots of matrices.

The second main approach adopted over the years to quantum chemical problems has been the use of "semi-empirical" methods, which sought to correlate different experimental results by an interpretive application of the wave equation. In this way results obtained from a range of molecules could be used to anticipate properties of further systems. This semi-empirical approach led to many interesting predictions without, at first, the need for heavy hand computations, but of late semi-empirical quantum chemical investigations have tended increasingly to necessitate lengthy calculation, in particular, the extraction of latent roots of fairly large matrices.

During the last two or three years, electronic digital computers have been used by a number of groups for both non-empirical and also semi-empirical calculations. Certain technical reasons have made hydrocarbons particularly attractive as subjects for quantum mechanical studies, which have appealed in turn to the petroleum industry. Mention may be made, for example, of semi-empirical calculations of ionization potentials of simple aliphatic hydrocarbons, effected on EDSAC, and which can be applied immediately to the interpretation of mass spectrometric data.[8] Non-empirical calculations, of a very elaborate nature, and which could, in principle, lead to results of any usable accuracy, have been carried out, also on EDSAC, by S. F. Boys, with the aid of new mathematic techniques which at one stage involve using the computer to carry out extensive algebraic reductions. These techniques await application to larger hydrocarbon molecules, using the more powerful computers presently available. Non-empirical calculations of a rather less ambitious nature, as regards the accuracy at which they aim, are at present sponsored by U.S. petroleum companies, who gave their support last year to an international meeting on valence theory at which a resolution was passed requesting extensive electronic computing facilities for quantum chemistry.[9] In their application to these problems, the computer is used first to evaluate molecular integrals by one of several equivalent methods[10] that all entail the use of special mathematical functions, *e.g.* Bessel functions, computed from infinite series, recurrence relations, and so forth; the manipulation of surface harmonics; and often numerical quadrature.[11] The final matrix calculations represent standard applications of the computers throughout many industries, for which matrix programmes written initially for perhaps the aircraft industry can be taken over intact, without any further work, to chemical problems.

STATISTICAL THERMODYNAMICS

Molecular energy levels derived from experiment, *e.g.* spectroscopically, or from theory can be used to calculate thermodynamic properties by the methods of statistical mechanics. Such methods were used, in conjunction with hand computation, quite a while ago, in connexion, for example, with the thermodynamic effects of internal rotation in aliphatic hydrocarbons. Several computers have been programmed recently to calculate "partition functions" from data concerning molecular energy levels, *e.g.* SEAC.[12] The various quantities such as free energies, entropies, and so forth can be found from these partition functions by simple formulæ. The partition functions themselves are basically the sums of exponentials of all energy levels possible for the molecules, scaled by a temperature factor. Partition functions obtained in this way require modification by further factors which accommodate intermolecular forces when these are significant.

The energy of a molecule can be split into three parts, electronic, vibrational, and rotational, each of which is quantized, that is to say, capable of assuming only certain separate well-defined values. These correspond to different integer values of the appropriate "quantum numbers." The rotational energy is determined by the molecular geometry (actually the moments of inertia) in conjunction with the quantum number. The vibrational energy is determined by the force constants that measure the forces which oppose distortion of the molecule from its equilibrium configuration, again according to quite simple formulæ. If the rotational and vibrational energies were independent of each other and of the electronic structure, the partition function could be factored into separate terms, one for each type of energy. The vibrational state, however, does have an effect on the rotational energy, and vice versa, and both are affected by the electronic state which changes both configuration, and hence moments of inertia, and also force constants. It is because of these interactions that programmes such as that just mentioned tend to become rather complicated. They permit the computer, however, to calculate rapidly extensive tables of thermodynamic properties, *e.g.* of hydro-

carbons over a range of temperatures, when provided initially with values of the basic parameters entering into the energy expressions.

COMBUSTION THEORY

The overwhelming use of petroleum products is as fuel in one or other type of moving or static source of power. It is doubtful if this situation will be changed for a very long time, if ever, even by the advent of atomic power, on the one hand, and the expansion of the petroleum chemical industry, on the other. The process of burning fuel has been the subject of much speculation and experimentation—a fuller understanding of this subject could well lead to the readier development of fuels which were more effective under particular conditions of operation. The mathematical study of flames, combustion, ignition, and related processes has expanded very greatly over the last few years, partly as a result of interest in jet engines and rocket propulsion, and partly as a result of the aid offered to this work by electronic computers. Combustion theory calculations are carried out to predict, for example, the limits on the composition of a mixture which can support a stable flame, *i.e.* which will neither explode nor extinguish, once ignited. It is convenient to treat such problems in terms of a static flame and a moving gas. Corresponding to any set of conditions such as composition pre-flame temperature and so forth, the speed of gas flow that will permit of a static flame is calculated. The non-existence of such a speed indicates the impossibility of stable burning under the specified conditions. Flames have as yet to be idealized to permit of any mathematical attack—turbulence and other sources of inhomogeneity being ignored. The combustion mixture is treated as continuous and varying in properties only along the direction of flow—this implies a laminar structure for the flames. The precise form of the chemical reaction affects the equations being solved only in its effect, as a function of temperature, on local gas density and further heat production. This information can be derived from the thermodynamics of the reaction. The actual calculations take into consideration conservation of matter, diffusion, heat creation and transfer, and ordinary hydrodynamic effects. In one standard approach [13] they amount to solving systems of partial differential equations, with time and the direction of flow as independent variables, and temperature and density as dependent variables. The equations need a computer for convenient solution (the CPC and 701 have both been used for this type of work). The equations are recast in difference form, each dependent variable in turn being integrated with respect to distance for one fixed time, the time variable then being stepped, and the process repeated again and again until the necessary time period has been covered.

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THE APPLICATION OF DIGITAL COMPUTERS TO PROBLEMS OF PROCESS DEVELOPMENT IN THE PETROLEUM INDUSTRY *

By J. T. AHLIN †

THE scientists and technologists of the petroleum industry have certain well-defined objectives in the application of engineering practices to refinery process development. Fundamentally, the objectives are concerned with the development, design, and study of processes towards the end of efficient, flexible, and economic manufacturing capabilities. One of the significant developments in recent years in the petroleum industry has been a systematic determination of the amenableness of these objectives to analytical solution utilizing the automatic digital computer.

The resulting engineering and technological accomplishment and associated economic success is measured not in terms of manpower savings, but rather in earnings brought about by improved process development and plant operation. An examination of the contents of trade journals and of the agenda of professional and society conferences indicates that the application of the electronic computer maintains a

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high level of interest in the petroleum industry. It is, therefore, pertinent that a progress report on existing areas of application be expanded to include a discussion of the motivation underlying the utilization of computers, as well as anticipated trends toward future development.

The basic motivation naturally follows from a desire on the part of process scientists to do an increasingly better engineering job. The attainment of this objective requires a better understanding of physical processes and a more realistic use of available data. The manipulation of voluminous files of data for purposes of better understanding the fundamental relationships between the variables with which the process engineer must concern himself is well suited to mechanized data processing. An understanding of the basic relationships between variables, even though the understanding may not be complete, permits the engineer to simulate processes and thereby utilize parameter variation techniques to design process equipment. It is the approach of design by mathematical simulation, which is so well suited to machine computation, that is the real impetus to the extended utilization of the digital computer in process development. The fact is that the digital computer has given the process engineer a new breath of ability. He is not able in most instances to mentally correlate the interaction between changes in the variables with which he is familiar. Only through the use of a high-speed computing device is he able to realize the full extent of his technology and to fully utilize the information which is available to him.

The computer has found important application in determining the consequences of a set of proposed unit design configurations. Yet, the same techniques have offered another, albeit often underrated, advantage. The digital computer is a worthwhile and necessary learning device. The fact that a computer is available to an engineering group means that routine applications can be mechanized and that the entire technology can be systematized. Thus, time and technique are available for an accelerated attack on new areas of engineering interest. Historically, the computer has functioned as a catalyst, in that the computer has stimulated its own utilization to the end of increasing process development and operational benefits.

The characteristics of the computer which have permitted and enhanced extended application are of interest. The most significant recent developments in computer technology are those concerned with electronic switching and the stored programme. Electronic switching devices have contributed speed and reliability. The stored programme has contributed a new ease of use and added greatly to the area of feasible engineering application, while, at the same time, maintaining the general purposefulness of its digital predecessors. Beyond these computer advantages are factors of storage capacity, accuracy, and input–output balance with arithmetic speed. But the success of computer application extension belongs essentially to the expanded area of potential application and the ease of computer use brought about by the stored programme concept and the development of new coding techniques such as the interpretive routine. These factors have made a company's computing facility available as a convenient service to engineers, who represent an increasingly larger amount of an organization's engineering activity. As an example of such widespread utilization, one refinery has run thirty-one applications, each with a different job description, during a typical day.

It is the purpose of this paper to discuss the application of digital computers to the problems of process development. The scope of process development with respect to computer application logically extends beyond laboratory and pilot plant investigations and the design of unit process equipment. The study of the performance of existing units for purposes of improving operation and suggesting design changes is also within the realm of process development problems. Indeed, the implementation of technological knowledge, which follows from performance studies on existing plant equipment, is an essential adjunct to the development of improved processes required for future expansion. Furthermore, the evaluation of an individual chemical engineering unit must be made within the framework of its environment so that the area of computer application to the understanding of plant operations must be added to the scope of process development problems.

On this basis, applications are described in the following areas:

(1) laboratory analysis;
(2) pilot plant operations;
(3) process design and mechanical engineering computations;
(4) finished process performance studies;
(5) unit improvement in operation and design.

The principal application of the digital computer in the laboratory phase of process development is associated with the desire to represent relationships between variables. Much of chemical laboratory research rests upon empirical data. The statistical treatment of data is well adapted to computer mechanization. Actually, standard programmes are available on most computers for least squares fitting, regression analysis, and variance analysis. The existence of these techniques and the ability of the computer to accommodate the simultaneous analysis of many variables has been of invaluable assistance in the design of experiments, for example.

An application of daily activity is the calculations associated with the reduction of mass spectrometer

data. The speed of inversion of the calibration matrix on a digital computer has altered the basic method of calculation in many instances. As an example, a 20th order matrix can be inverted on the IBM 650, using a method of elimination and floating decimal subroutines, in ten minutes. It is, therefore, feasible to invert calibration matrices following each recalibration of the mass spectrometer and utilize an efficient matrix by vector multiplication for the daily determination of sample component percentages. One IBM 650 mass spectrometer programme computes:

(1) an observed peak height from an apparent peak height and scale factor multiplication;

(2) a sum of partial pressures without check peak contributions;

(3) a sum of partial pressures without check peak contributions and with negative partial pressures set to zero;

(4) a sum of partial pressures without check peak, negative partial pressure, and water and air contributions;

(5) the molecules per cent of each component.

These calculations are performed at approximately 200 samples per hour for an 18 component, two check peak sample, and 150 samples per hour for a 25 component, two check peak sample. Previously, approximately 30 minutes per sample was required using manual methods. A typical laboratory may process 40 samples per day.

Recently, an involved series of trial and error computations on the IBM 650 led to the establishment of a simple, straightforward analytical technique for the determination of the composition of metal and other deposits. The data had been gathered by subjecting the deposits to X-ray fluorescence. It is believed that this technique could not have been developed without the assistance of a high-speed computing device. Certainly, the ability of the digital computer to mechanize flash calculations, distillation, absorption, and stripping computations has played an important role in laboratory analysis. Several other laboratory applications are of interest. The application of the statistical determination of experiments, the control of laboratory samples, and the establishment of a library cross-referencing file using randomly punched cards have been mechanized. Another area of process development that has been found to be well adapted to machine computation is the work-up of pilot unit and plant test data. The conversions of meter readings, physical properties, and meter characteristics to flow rates have been mechanized. In addition, the calculation of qualities and yields of products from various streams and the correlations of other useful relationships are computed as a normal part of a machine procedure. One refinery pilot plant organization found that attempts to conduct tests on a multi-variable unit, wherein all but one variable was held constant, were unsatisfactory. Employment of the ability of the digital computer to perform regression analyses and methods of steepest ascent permitted this group to obtain more useful results from existing data and to modify its basic philosophy on the design of experiments.

The design of a process is a natural outgrowth of the ability to stimulate mathematically the process itself. The computer is not capable of carrying out design directly, but merely examines a predetermined set of specifications and establishes the consequences of a proposed design. The capacity of the digital computer to explore manifold proposed designs, coupled with the engineer's experience and imagination, makes possible an improved design in many cases. Several examples of design improvement in the petroleum industry have been attributed to the computer's ability to give a more complete parameter functional. Often by the device of parameter variation, improved and rational designs have been suggested which would have gone undetected in a study of lesser magnitude. Distillation programmes, using plate-to-plate techniques, which have been written for purposes of control, have served as a basis for design studies. This is merely one of many areas wherein a process simulation method derived for performance or control purposes has aided the process designer.

Many mechanical engineering design applications have been mechanized. Invariably, these calculations represent more rigorous solutions to problems formerly solved using short-cut methods. Typical among these are vessel and flange stress calculations, the determination of economical thickness of insulation, and pipe stress analysis. Pipe stress calculations, using methods such as the Kellogg method, are rarely done using hand methods. An IBM 650 programme which utilizes this method has been written. The programme computes the combined stresses at both ends and the midpoint of every bend or elbow and at the anchors, for either a 2- or 3-anchor line. Both hot and cold anchor reactions are also determined. Running times for a 2- and 3-anchor problem are approximately 6 and 12 minutes, respectively. One estimate indicates that the 2-anchor problem done by hand methods utilizing the Kellogg method would require 20 hours.

A combination of previously discussed techniques permits the engineer to study the performance of the finished process. The accumulated understanding of the new process makes possible operation and design improvement on the unit as well as giving insight into the design technique which the finished product represents. Indeed, performance studies indicate methods of improving the operation of a chemical engineering unit, as well as suggesting immediate design changes.

Several types of process have been subjected to

careful analysis utilizing computer facilities. One of the most active areas of process study is the solution of multi-component distillation problems using plate-to-plate techniques. An IBM 650 distillation programme which represents a completely integrated, flexible, and rigorous approach to the solution of multi-component distillation problems has been widely used. The programme is written to handle all initial assumptions, data conversions, preliminary and set-up calculations, adjustments, and terminal calculations in a single computer run. The programme handles sharp as well as sloppy separations and is capable of rewriting parts of itself to cope with a wide variety of special requirements. The computation technique includes such refinements as complete heat balances around each stage, the evaluation of equilibrium and enthalpy data at true tray temperatures, and automatic feed-plate matching. The programme will handle a maximum of 20 components and 98 theoretical trays. One user duplicated the equivalent of four man-years of computing effort in two weeks using the programme. A typical problem with 15 components and 40 plates can be set up and run in less than a day. Additional work-ups utilizing the same feed data can be run in two hours of computing time.

Substantial improvements have been made by several organizations in the methods of obtaining and processing unit correlations through the use of computing and statistical techniques. The catalytic cracking unit has received considerable attention as a likely area for process improvement. Increased catalytic cracker product value employing computing and statistical methods has been measured in cents per barrel in several refineries. Motor gasoline blending has also been established as a routine computer application in several instances. The problem of determining an improved economic method of blending twenty components, for example, to produce desired amounts of various grades of gasoline is being undertaken using computer linear programming programmes. An optimum blend appears to require new mathematical methods of non-linear programming or a trial-and-error approach wherein a linear programming solution is obtained for each trial. However, the computer solutions to date have indicated earnings through linear programming blending amounting to as much as 2 cents per barrel. This earning is of further significance in that the linear programming solutions are obtained in less than one hour per day using a digital computer such as the IBM 650.

Additional computer applications in process development exist in unit operation improvement. Yet, unit studies have full meaning only as a portion of plant performance studies. The simulation of a refinery permits a realistic evaluation of a process within its frame of operation. It is interesting to note that the refinery simulation application which encompasses the objective of unit simulation within the unit's environment has met with success. Refinery simulation has been accomplished in at least two cases utilizing the IBM 700 Series equipment. One of these, a fully automatic procedure, includes distillation to specified cut points, visbreaking, catalytic cracking, thermal cracking, blending, fuel disposal, and the calculation of costs, profit, and a material balance for checking purposes. In addition, several refineries have been simulated on intermediate digital computers. Refinery operating plans have been evaluated on the IBM 700 Series machines in from 10 minutes to one hour per plan. The IBM 650 simulation programmes ordinarily run in excess of an hour.

The amenableness of the digital computer towards meeting the objectives of the petroleum process engineer is established at all levels of process development in the petroleum industry. Fortunately, the academician and the industrial researcher have developed and are developing mathematical techniques for the solution of partial differential equations, for the study of physical and chemical systems by Monte Carlo methods and linear programming, and for the formal representation of models for simulation purposes which have gone hand-in-hand with the development of the digital computer. With these mathematical tools and with the imagination and ingenuity which characterize the process engineer, the future application of the digital computer in process development is certain to undergo continued growth. A projection of experience to date indicates that the computer will find utilization as a necessary tool across the entire spectrum of process development, from the smallest laboratory glass experiment to the complete refinery simulation towards the end of an improved product at less cost.

THE APPLICATION OF A COMPUTER TO REFINERY PROBLEMS*

By B. D. DAGNALL† and P. MAYERS†

SUMMARY

Two types of application are described by reference to two actual examples. One, an operating problem, is the calculation of the optimum operating conditions of a plant, the other, a management study, is the simulation of the operation of proposed new equipment by computer.

INTRODUCTION

THIS paper does not discuss accounting applications, which are the subject of many references, or routine jobs such as mass spectrometric calculations,[1] which raise no novel points. Two types of application will be described, both of which may save a large amount of money but need only a simple computer, and neither of which are peculiar to the oil industry.

The first problem is the determination of the operating conditions of a plant so that the performance is in some sense best. One is not concerned here with the definition of "best"; it will merely be assumed that in an actual problem the performance of the plant can be measured by one number, which will be called the response. It will probably be a function of quantity and quality of the products and of the cost of operation. If correctly defined, the profit may be used as a convenient measure of the plant's performance. The problem then is to maximize the profit.

The second application is the use of a computer to simulate the operation of some proposed new equipment under a variety of conditions in order to provide management with information which will enable it better to answer the questions "How many?" or "How big?" when considering the provision of new facilities. In a few hours the computer may well simulate several years of operation of a piece of equipment which exists only on paper.

THE DETERMINATION OF BEST OPERATING CONDITIONS

In running a complex plant, such as a catalytic cracking unit, it may be highly desirable to know, but difficult to determine, the conditions of operation which give the required products of the requisite qualities at lowest cost.

In general, it is not possible to start with product requirements and by the rules of arithmetic to calculate the necessary operating conditions. (The method of linear programming[2, 3] does this in certain cases, but the large number of variables which arises in practice, and the condition of linear relationships between the variables, considerably limit the value of the technique.) Usually all that can be done is to assume some operating conditions and by lengthy and tedious arithmetic calculate the effect of these conditions. To solve the problem, therefore, it is necessary to perform this lengthy calculation a number of times with different assumed conditions. Furthermore, it is desirable to choose the series of assumed conditions in such a way that the solution is obtained in the smallest number of trials. The way of doing this which appears most promising to us is the method of Box and Wilson,[4] which will be described. The whole problem thus falls into three parts:

(1) Determining the rules from which the performance may be calculated from the operating conditions. This is known as setting up the mathematical model.

(2) Devising a computer programme to do this calculation.

(3) Selecting each set of trial conditions, by reference to earlier results, to get as big an increase in response as possible.

THE MATHEMATICAL MODEL

The model of the catalytic cracker consists of a set of correlations specifying the effect of each variable on the products. These are based on theoretical grounds and on the past performance of the plant. Before use the model should be tested, if possible, by checking its results against known ones. Even if agreement is poor the model may still be useful to give comparative results and not absolute ones, as results from a poor model may be numerically in error but directionally correct.

THE COMPUTER PROGRAMME

The correlations must be put into a form suitable for computation. This involves, for instance, replacing graphs by polynomials, and feeding in tables so that the number of tabular entries, and the order o interpolation needed, are fitted to the store and speed

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of the machine. The use of floating-point arithmetic, in which all numbers are expressed in the form of $a.10^b$, where a lies between -1 and $+1$ and b is an integer, simplifies the coding; whether to adopt it or not must depend upon the particular application and the features of the computer.

Programmes have been made at Fawley for both the catalytic cracker and the hydroformer. The first, working in fixed-point arithmetic, takes an hour and a quarter running time on a HEC computer. The other, using floating-point, takes about twenty minutes.

THE METHOD OF STEEPEST ASCENTS

To illustrate this method a simple example will be taken. Assume that from the performance of the catalytic cracker the profitability of the operation can be calculated. Suppose also that in a particular study it is desired to find the values of the following four variables which give the highest profit:

(1) feed rate, F, measured for convenience in hundreds of barrels a day;

(2) reactor temperature, T, in ° F;

(3) catalyst proportion, C, in pounds of catalyst to pound of oil;

(4) catalyst activity, A, measured by percentage $D + L$.

Now limits on the values which each of these can take are imposed by plant limitations and by knowledge of the performance of the plant. The more the range of variability can be limited by prior knowledge, the quicker the optimum solution will be obtained. For illustration it is assumed that the limits given in Table I apply. (This particular example is hypothetical and does not give actual Fawley values.)

The best estimates of the operating conditions might be $F = 450$, $T = 900$, $C = 10$, and $A = 30$, and these will be used for the starting point. With these initial values the computer is used to calculate the response, which in this case is the profit. It is found to be 509 (in quite arbitrary units). The question now is, how should the four variables be altered so that the increase in profit P is likely to be as large as possible? It may be shown [4] that this is the case if each variable is increased in proportion to the partial derivative of the response (profit) with respect to the variable. The partial derivative is merely the increase in response if the variable is increased by one unit. The calculation of the four derivatives, 5, 4, -5, and -9 is shown in Table II. This involves four runs on the computer. In the determination of dP/dF the variable F has been increased to 451, which is beyond the upper limit of 450. Providing the correlations apply for this value, this is all right, as one is not specifying that the feed rate can be 451 but is only obtaining the rate of change of P with F for $F = 450$.

TABLE I

Limits of Operating Conditions and their Initial Values

Variable	Units	Lower limit	Upper limit	Initial values
Feed rate, F . .	Hundreds brl/day	300	450	450
Reactor temperature, T .	Degrees F	850	950	900
Catalyst proportion, C .	Pounds per pound	5	15	10
Catalyst activity, A .	Per cent $D + L$	20	35	30

TABLE II

Selection of Step Size for First Ascent

Variable	Starting point	Unit increase in:			
		F	T	C	A
F . . .	450	451	—	—	—
T . . .	900	—	901	—	—
C . . .	10	—	—	11	
A . . .	30	—	—	—	31
Profit, P . .	509	514	513	504	500
Increase in P .	—	5	4	−5	−9
Step size . .	—	1	1	−1	−2

The absolute increases in the values of the four variables is a matter for discretion; it is necessary only to preserve the correct ratios between them. It might be decided to try the increases 1, 1, -1, and -2 respectively, which are convenient sizes proportional to the derivatives. This selection of the size of the step is not done by machine but is left to the human operator, as it is a question of judgment. It is now possible to "make the first ascent" as it is called. Applying these increases, subject to the variables not exceeding their limits, the profit is calculated by machine to be 529, which is an improvement on the first value of 509. Another step is now taken by repeating this operation, obtaining a profit of 539. A third step gives a profit of 540, and it may be guessed that a fourth step would give a lower profit. These results are summarized in Table III. Nothing will now be gained by taking another step with these same increments. New partial derivatives now have to be calculated (Table IV), step sizes chosen, and a second ascent made (Table V). After step 3 it is realized that further steps lead to a reduction in profit and step 2 is used, giving a profit of 578 units, as a starting point for the third ascent (Tables VI and VII). Proceeding in this way (Tables VIII and XI), a stage is reached where it is decided that the profit increase to be obtained by further ascents does not justify the work involved, and the values $F = 450$, $T = 920$, $C = 7$, and $A = 25$, giving a profit of 623 units, are accepted as the best operating conditions.

The terminology of this process is based on finding the summit of a hill. The process involves selecting the steepest ascent from the starting point, taking a

number of steps in this direction until one begins to go down again, and then changing direction. Eventually one will either get as near the summit as reasonably matters or will reach the top of a minor hump on the side of the hill. Fortunately the analogue of a minor hump in running a chemical plant is unlikely to arise.

A study of Tables II to XI justifies criticism of the selection of step sizes and at which step a new ascent was started. For instance, a graph of profit against step number (or examination of second differences) suggests that in each of the first three ascents it could have been anticipated after step 2 that a further step in the same direction would give no large profit increase, and that it would have been more economical of time to have omitted the third step. There is also a suggestion that the profit is very sensitive to catalyst proportion and that a smaller unit should have been used, for instance, ounces of catalyst per pound of oil. One of the values of a computer in a study of this nature is that as well as solving the main problem it throws light on the effect of each variable on the performance of the plant.

TABLE III
The First Ascent

Variable	Starting point	Step 1	Step 2	Step 3
F	450	450	450	450
T	900	901	902	903
C	10	9	8	7
A	30	28	26	24
P	509	529	539	540

TABLE IV
Selection of Step Size for Second Ascent

Variable	Starting point	Unit increase in :			
		F	*T*	*C*	*A*
F	450	451	—	—	—
T	903	—	904	—	—
C	7	—	—	8	—
A	24	—	—	—	25
Profit, *P*	540	546	545	541	543
Increase in *P*	—	6	5	1	3
Step size	—	6	5	1	3

TABLE V
The Second Ascent

Variable	Starting point	Step 1	Step 2	Step 3
F	450	450	450	450
T	903	908	913	918
C	7	8	9	10
A	24	27	30	33
P	540	569	578	576

TABLE VI
Selection of Step Size for Third Ascent

Variable	Starting point	Unit increase in :			
		F	*T*	*C*	*A*
F	450	451	—	—	—
T	913	—	914	—	—
C	9	—	—	10	—
A	30	—	—	—	31
Profit, *P*	578	582	582	575	569
Increase in *P*	—	5	5	−3	−9
Step size	—	2	2	−1	−3

TABLE VII
The Third Ascent

Variable	Starting point	Step 1	Step 2	Step 3
F	450	450	450	450
T	913	915	917	919
C	9	8	7	6
A	30	27	24	21
P	578	604	610	596

TABLE VIII
Selection of Step Size for Fourth Ascent

Variable	Starting point	Unit increase in :			
		F	*T*	*C*	*A*
F	450	451	—	—	—
T	917	—	918	—	—
C	7	—	—	8	—
A	24	—	—	—	25
Profit, *P*	610	614	615	611	612
Increase in *P*	—	4	5	1	2
Step size	—	4	5	1	2

TABLE IX
The Fourth Ascent

Variable	Starting point	Step 1	Step 2
F	450	450	450
T	917	922	927
C	7	8	9
A	24	26	28
P	610	620	590

TABLE X
Selection of Step Size for Fifth Ascent

Variable	Starting point	Unit increase in :			
		F	*T*	*C*	*A*
F	450	451	—	—	—
T	922	—	923	—	—
C	8	—	—	9	—
A	26	—	—	—	27
Profit, *P*	620	622	618	619	619
Increase in *P*	—	2	−2	−1	−1
Step size	—	2	−2	−1	−1

TABLE XI
The Fifth Ascent

Variable	Starting point	Step 1	Step 2
F . .	450	450	450
T . .	922	920	918
C . .	8	7	6
A . .	26	25	24
P . .	620	623	612

SIMULATION OF THE OPERATION OF NEW EQUIPMENT BY COMPUTER

When the provision of new facilities is under consideration it is often difficult to decide on their extent because of the fluctuations in the demand on the facilities. The average demand is of little use, the need being knowledge of the incidence of high demand, so that the loss incurred when the facilities are inadequate may be compared with the cost of additional facilities. The obvious example is the case of stocks where the size of the stock should be such, not that any conceivable demand can be met, but that the cost of holding additional stocks exceeds the loss suffered on the occasions when the item is needed but not in stock. It is in giving some measure of the fluctuations in demand for the facilities that the computer can be of use, especially where the fluctuations are due to random effects such as weather.

To illustrate this application, a hypothetical example based on one of the most costly stores items, namely stock of crude oil, is considered. Assume that extra crude distillation facilities are being provided and that the tanker fleet is being suitably enlarged. The problem is to decide on the number of extra crude storage tanks needed. The stocks to be held depend upon:

(1) variations in the crude distillation rates;
(2) schedule for tank inspections;
(3) variations in the intervals between arrival of tankers;
(4) variations in the loads of the tankers.

Assume also that the problem has been studied and that estimated frequency distributions have been made of each of the above factors. The questions that management want answered, for a given number of tanks, are:

(1) How often, and for how long, will there be no stocks of crude oil available?
(2) How often, and at what cost, will tankers be held up because there is no available tankage to discharge into?

As before, a mathematical model and a computing scheme are set up such that, over a given time interval, if the crude withdrawal rate, the times of arrival of tankers in the interval, and their loads are known, the change in stocks can be calculated and totals accumulated of the time during which stocks were exhausted and the time tankers had to wait. (There is nothing difficult about this calculation; it could easily be done by hand, but when the use of the tanks over a period of years under various conditions needs to be investigated it becomes too tedious to be done by hand if a computer is available.) All that is needed now is a procedure whereby the machine generates a series of crude distillation rates, intervals between tanker arrivals, and loads, each of which fits the appropriate frequency distribution, and runs through the basic calculation. This generation of a series of values fitting a specified frequency distribution may be accomplished by the machine's ability to obtain a random number and look up a table.

Thus, if the number of tanks, the initial stocks, and the appropriate distributions are fed into the computer, the operation of the tanks over a period of years can be studied by the machine, and the numerical answers to the two questions obtained. As before, the model must be tested against known results. A number of runs for different conditions will give a good indication of the risk of running out of crude, and of the tanker waiting time, for any number of tanks. Thus, a series of trial runs on a pilot plant which does not exist have in effect been done.

JUSTIFICATION OF A COMPUTER

This application is not spectacular, it does not do the work of hundreds of clerks, it does not involve the use of mathematics, and it does not produce answers which could not possibly be obtained by hand. The application is easy to code and the simplest computer is suitable. Nevertheless, the results obtained might prevent the refinery running out of crude, might save expenditure of tens of thousands of pounds on unnecessary tanks, or may only confirm that conclusions reached by other means are probably right. It is characteristic of many computer applications that the value of the results it produces cannot be determined in advance; to know the savings it is necessary to know the answers it will produce to specific problems. Thus, justification for a computer in financial terms cannot usually be made in advance. All one can say is "here is a tool which costs x pounds, it may save us no money, it may save us hundreds of thousands, let us try it."

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DISCUSSION

D. A. Glen: I must confess myself as being one of those converted to the thought that the computer is going to be of tremendous value in our industry. One of the first things one discovers is that it is not a question of its being of value in one specific field, but in an extraordinary variety of fields.

We must be very grateful to Mr Dagnall and Mr Mayers, who have shown us a very practical application of the sort of thing that has already been done. The important feature here is the demonstration that these problems are in fact already being tackled by computers.

Dr Ahlin has mentioned that we have got to cast around for new techniques. It seems that this shows that the application of the computer to our problems divides into two spheres which perhaps overlap. First, the application in spheres in which the problems are already well formulated, *e.g.* in the scientific world, where one is accustomed to reducing problems to mathematical terms. Here the problem of computer application is the strictly practical one of working out answers faster and more efficiently than before. It seems that the computer is going to be of tremendous value to the industry in this speeding-up of operations, enabling a man to work in a given time for a better answer. Anybody who has anything to do with any kind of planning job, whether it is day-to-day operational or long-term planning, has at some time been faced with a massive jigsaw, and had to pick out bits from it and fit them together to make a pattern. It does not make much fundamental difference whether the pieces of the jigsaw are the refinery plant and the pattern a refinery, or whether the pieces are ships and the pattern a shipping programme. No doubt everyone who has done that kind of job has been left with a query in his mind as to whether he has really arrived at the best answer. The speed of the computer may enable him to try out more alternatives.

Secondly, one comes to the next sphere of application and to Dr Ahlin's very interesting remarks about new techniques. He referred to " the study of the problem in its environment " and the techniques for doing this. One has to be prepared to open one's mind to new ideas. An example which has been mentioned is that of linear programming. For the benefit of those who are not familiar with this technique, linear programming consists, in short, of setting out a problem in terms of mathematical equations together with, also in mathematical terms, a function which it is required to maximize. This done, the computer can be set to work, and, in effect, surveys the whole field of possibilities, ultimately choosing the solution which gives the maximum value to the function. In other words, if the mathematical model represents a refinery process, and the function represents the profit one wishes to maximize, then the solution given will be the most profitable way of running that refinery process. Working this way there are no worries as to whether the final solution can be improved upon.

There are limitations to the technique, and it is noticed that Mr Dagnall and Mr Mayers make particular reference to them. I would, however, like to hear more from Dr Ahlin as to whether these limitations are so severe. My early impression is that they are not because I have seen some quite successful sets of up to 200 equations handled by linear programming on the Ferranti computer at the Royal Dutch/Shell Laboratories. 200 equations seems to be a number with which one can begin to work out quite a tolerably accurate model.

There is just one other point, and that is the question of the speed-up of the processing of data; the collecting and collating of all the raw figures of industry, which have to be welded together to form the financial and statistical statements that are so essential to efficient management. Every one of us has probably had the experience of working on figures that are known to be already out of date.

C. M. Berners-Lee: We, in the U.K., are a long way behind the Americans, but in one or two small groups some very fine work has been done, and our conclusion from operational studies is broadly the same as Dr Ahlin's: that a computer is a very fine learning tool.

In regard to linear programming, the work which has been done on the Ferranti Mark I computer in Amsterdam has shown that one can tackle very significant problems on a computer. The linear programming type of problem can be tackled only because, in fact, one does not have to examine all the possibilities. The linear programming technique enables one to find the best solution to the problem by a process which is similar to that of climbing up the side of a mountain. This mountain is like the one in the earlier example, except that it has sharp edges formed by the intersection of plain faces. The climb starts from the bottom of the mountain, and one climbs up the ridges until one gets to the top, without visiting all the possible vertices of the mountain. The fact that there is an important class of problems in which one can reach the optimum solution in this way is a great help, and there is a number of real problems which can be fitted into the linear programming model. However, there is also a number which cannot be fitted into this model, and where one is faced with either attempting to examine all the possibilities, or to look at only some of them. It is very easy to set a computer a completely impossible task. For instance, if one thinks of the streets of London as being a mesh of sixty streets north and south, and sixty streets east and west, and if one wants to get from one corner of the mesh to the diagonally opposite corner, there are about 260 ways of doing it. If one knew the time it took to get down each street, theoretically this could be solved, but in practice this would keep any computer going for the whole of its life, and it still would not have got there at the end of it. This difficulty can be got over in a lot of cases; one can devise a technique which does not give the best solution, but which gives a solution which is not too bad and is probably very considerably better than anything that can be done by manual methods, simply because very many more possibilities can be examined. The U.K. is still a long way behind the U.S.A., but a start was made when there was a conference on linear programming in 1954, and since that time quite a lot of work has been done on linear programming problems in this country for other industries, and abroad in the petroleum industry.

P. B. Coaker: In regard to the paper by Mr Dagnall and Mr Mayers it is my personal understanding that the method of Box and Wilson, which the authors have used, was really developed for use as an experimental technique for the optimization of unit operations. With a given unit one would design an experiment in which the conditions were varied about a fixed point, and from the results of this experiment one would calculate the line of steepest ascent. By doing further experiments

along this line one would progress successively towards the final optimum. In the quoted application the authors have used a known correlation and have applied the method of Box and Wilson to this. I would like to ask whether it would not have been possible, having obtained a correlation, to differentiate this analytically, thus arriving at the optimum directly. If the correlation was complex I can envisage that it may be necessary to differentiate it numerically, but I would have thought that by doing this it would be possible to arrive at the optimum in a complete calculation which occupied only one computer run. In the method quoted it seems that the computer is used on short runs only and that there is a large amount of data transfer to and from the machine between runs, a technique which cannot utilize the machine to its utmost efficiency.

The second point concerns the reference to linear programming. I have been investigating the technique of linear programming, and one fact that emerges is that one cannot consider the profitability of a single unit in a refinery without considering the profit made by all the other units. I agree that it is difficult to apply linear programming techniques when one has non-linear relationships, but it is possible by using a series of linear approximations, although this may lead to a prohibitive number of equations. I would like to ask the authors whether they consider, and if so how they consider, the profitability of the catalytic cracker in combination with the operations on all the other units within the refinery. To illustrate the question, in the problem of the catalytic cracker operation the optimum profitability was obtained with maximum feed rate. This high feed rate will give a large quantity of products, which it may not be possible to blend with the components available from the operations on the other units. Hence one has made a profit on the catalytic cracker, but a consequent loss in the blending programme. Thus both operations must be considered concurrently. Similarly, if one has other units which provide high octane components, the operation of these units must also be considered with the operation of the cracker.

The two questions I have to put to the authors are therefore: (1) are they considering the profitability of the cracker in combination with the other units on the refinery? and (2) was there any particular reason why they used the method of Box and Wilson for their optimization, rather than an analytical method?

P. Mayers: On the question of profitability, naturally one has to consider the operation of the cracker in relation to one's requirements. It is no good running the plant at an enormous feed rate, and producing large quantities of unsaleable products. One has to consider the whole thing. This is almost getting into the field of complete refinery simulation, and we are making steps along that road, but it is going to be a much more difficult problem.

As to the optimization, the technique of Box and Wilson was used because it seemed fairly simple, once it was understood, and I dare say one could make the machine choose its own points for the next ascent, but unfortunately our machine is not large enough for the job. It is easier to get the results out into the air, examine them by handling, and then start off again.

We feel it is quite valid to use the Box and Wilson method, even though its original purpose was the design of actual experiments. Instead of performing a physical experiment we are substituting the prediction of results by the computer programme and using these results for the design of further "experiments."

P. B. Coaker: You are in fact saying that you use this particular method because of the size of your computer, that you could not cope with a larger programme because of lack of storage capacity.

P. Mayers: It is thought that one would need a considerably larger programme in order to cope with an internal organization technique. We did think of it, but due to the difficulties on the machine itself, it is just as simple to do that step by hand.

Ph. Dreyfus: I would like to ask Dr Ahlin if he knows of any applications where real time control of refineries is achieved with the help of high-speed computers such as the 704.

Dr J. T. Ahlin: There are at the moment no 704's installed in the U.S. petroleum industry. Furthermore, to the best of my knowledge there are no large real time petroleum applications in existence. However, there are a considerable number of real time applications in other industries in the U.S.A., especially in guided missiles work, which involves some sort of tracking device. I feel that because of the fact that the basic time cycle in a refinery is considerably less, or slower, than in other processes, such as a missile simulation, a jet engine test study, or wind tunnel studies, that the problem of real time simulation in a refinery becomes considerably more practical, and I suspect that it is only a matter of time until this is actually done.

We have just begun to have a feeling for the problem of coupling instrumentation and computers, with feedback mechanisms which will make this possible. There are many problems involved, but it will not be long before there will be some very significant real time applications in the petroleum industry.

M. E. Weinstein: I should like to ask whether there has been any experience in the U.S.A. in the use of digital electronic computers on the marketing side. There are problems in the U.K. which involve the processing of data amounting to over half a million items, which in the course of their passage through the marketing machine may be re-recorded anything from seven to fourteen times. It would be interesting to know of any developments there might have been in handling data on this scale. It does not, of course, involve complicated mathematical calculations upon a small amount of original data, but is much more the carrying-out of the simpler calculations which one makes in marketing statistics, such as comparisons with a previous period or with other areas and so on, in relation to a vast number of separate items. In addition, there is a particular interest in the ability to feed into the machine certain instructions which would define limits of variance from some kind of designated norm, such as the national or average market appreciation, and confine further analysis only to those items which may vary by, say, 5 per cent on either side of that central line, so that it is not necessary to process a great volume of items in the machine. One would, however, want to take out quickly all those variations which were greater than this 5 per cent either way. Has anything been developed along those lines in the U.S.A.? So far as my knowledge goes, in Britain nothing has yet been worked out in practice.

Dr J. T. Ahlin: Several companies have attempted to determine the location of retail gasoline stations in new marketing areas on the basis of various factors which they feel are significant to the sale of gasoline and other products ordinarily purchased in a gasoline station.

There is a very good precedent for this in that one of the largest manufacturers of automobile accessories, mainly making seat covers, has conducted some very significant studies and adapted the results of these to determine where retail outlet stores should be located. This was done by considering many things which could be thought of as affecting the sale of seat covers. The factors which come to mind are such things as the average age of cars in the vicinity, the local income classes, and the closeness of competitive stores. This organization made a very exhaustive study, using the Service Bureau 701 in New York, and were able to narrow down the number of variables to a lesser number of key variables, and on the basis of these correlations were able to draw iso-sales potential lines on maps. Once this was done and the map completed, some interesting results were obtained. The organization wanted to locate essentially at the peak of these contours. There were problems which had to be handled manually resulting from this; for example, it turned out on occasion that the optimum location in a particular area was in the middle of a cemetery, so that other factors of suitability, zoning restrictions, and selling price had to be brought in.

M. E. Weinstein: I am thinking more of feeding-in or programming into the computer instructions which will determine a kind of planned average, or near average, marketing achievement. This can be in terms of whatever is considered appropriate, *e.g.* comparison with the same period of the previous year, or of the previous month, or with what is thought to be the appropriate share of the available market. If, then, one can hold in the machine all the results which conform within limits to this norm, one can proceed quickly to the analysis of those items which fall outside these limits.

Dr J. T. Ahlin: Is it correct to say that you are talking here on a sort of exception basis?

M. E. Weinstein: It might be better to put it this way. It is desirable to concentrate on things which are important from a marketing point of view to secure further information about good activities, and to learn more about them, yet on the other hand to take measures to put right weak elements. These are essentially the management problems in a marketing organization.

Dr J. T. Ahlin: I cannot speak specifically of any marketing application, but perhaps I could mention some inventory applications which are not dissimilar, since there are the same basic requirements. Certainly large inventory information is maintained, and it is subject to alteration by additions, deletions, and spoilage. Several companies have been doing this for some time now. They do include accounting by exception. Everything which is normal is examined by the machine and is passed by without any notification. However, all abnormal conditions are determined and, in addition, some resulting action is indicated. In one of these applications, involving an inventory, considerable information is kept on each part; not only information describing the part, but also where it can be purchased, where it has been purchased in the past, what the relationships have been with various suppliers, and even, in each case, the purchasing agent who handles the item. When the part becomes in short supply, a purchase order will automatically be printed with information concerning its previous purchase history and actually routing the information, so that this goes automatically to the man who handles it. Furthermore, a considerable amount of this work is being done in adjusting minimum inventory levels, and mathematical techniques are used there.

Dr M. P. Barnett: There are numerous market research applications of computers, although I cannot recall any in the petroleum industry itself. However, for many other commodities studies are made in which stock levels at successive times are processed on electronic computers. Sales figures for sample shops are blown up to regional values by multiplication with multiple weighting factors and an indication is given thereby of excessively high or excessively low sales. Tests are also applied within the computer to determine whether apparent trends are really significant in the statistical sense.

Ph. Dreyfus: Could Dr Ahlin comment on what has been done in the computer field with respect to tanker fleet scheduling?

Dr J. T. Ahlin: I would like to mention an application which is analogous to this, and which might give some idea of what is being done. This might be an extension of the question which was discussed earlier about linear programming. One would ordinarily ask what happens when linear programming is not applicable and when one has problems which seem to be in the same category? How does one approach and handle them? One technique, which is very impressive, is the use of Monte Carlo method. Although the term may seem strange, they are easy to understand and apply. The work under explanation has actually been done by Esso at Baton Rouge and has been written about.

The problem consists of determining tankage requirements at the refinery. The input to the tank farm is from a pipeline, and there are two possible outputs from the tank farm. First, crude can be processed in the refinery itself, or secondly, it can be transported by coastal tanker to East Coast refineries.

Therefore crude is coming in by pipelines; some of it can be processed in the refinery, or the excess can be taken away by tankers. In this case crude arrived in excess of the ability of the refinery to process it, so there was always a minimum tanker requirement. The question was: how could the amount of tankage needed to cope with the fluctuations in this particular system be best determined? The fluctuations were brought about by the fact that crude would arrive through the pipeline in varying amounts on a daily basis about a long-range purchase plan. Another fluctuation in the system was that the crude which could be taken into the refinery first had to be processed by pipe still, and the capacity of these stills to accept crude also fluctuated because occasionally one of them would be down for repair. Less frequently two or more might be down, so that the refinery capacity would be subject to fluctuation, and the tanker fleet, due to arrival of ships at random times, was also subject to fluctuation.

The company thus had a system about which it had historical information and which it wanted to study to determine tankage requirements. The question was, therefore, how to solve this problem? One might have taken the average crude coming in through the pipeline; taken the average refinery capacity, and the average tanker availability, subtracted the latter two from the first, leaving the difference to represent tankage requirements. It turns out that it is not very safe to work with averages. It is like the statistician who drowned crossing the stream which had an average depth of three feet. One might also think of a newsboy; he found yesterday that he sold forty newspapers, but this does

not mean that today he will have as many as forty requests, or that he might not have more than forty. It is merely a gauge and real-life situations are subject to fluctuations. A new technique was required, and the Monte Carlo technique was chosen.

The company was interested in determining a curve which related tankage requirements to tanker capacity. It turned out that there were certain minima here. One is that a minimum number of tankers was required, since the crude came into the system in excess of the refinery's ability to process it. Also required was a certain minimum amount of tankage.

What was done can be demonstrated by considering the pipe stills. It was necessary to determine the expected down-time for each pipe still, so historical information was gathered from each still. This was represented by a simple frequency distribution curve showing the number of days that the particular still had been on stream and another curve for the number of days it had been down. From these was formed an accumulated frequency curve. Curves were obtained for each pipe still, representing up-time and down-time, and it was possible thereby to determine, on the basis of actual expected behaviour, the number of days that each still could be expected to be available.

A still might be down for several days and another still might also be down for several days, so every once in a while there would be overlapping of down-time. Thus by summing availability for a particular day, one can get the total pipe still capacity, and hence determine the actual and expected amount of crude that the refinery could handle on any particular day.

The way this was done was quite simple. Curves were derived for each pipe still to represent the up-time and down-time, and then a random digit, between zero and 100, would be generated in the computer. Once that digit was found, the operator would go across to the curve, drop down, and read off the number of days that the still would be on stream. Another random number gives the expected number of days that the still would be down. Then the operator would go back to the first curve and repeat the process. This was done for each still, and capacity was summed up for each day. This technique permitted the company to actually get an idea of how much pipe still capacity it could expect on any day in a normal situation. The employment of this simple technique enabled it to get, for a fixed number of tankers, a distribution curve which represented the tankage requirements. One point would represent the minimum tankage, and another would be the amount needed to handle the worst possible case. Then the company would plot for that number of tankers, points A and B representing the minimum and maximum tankage requirement. This same model would be run for another number of tankers and two more points would be found. By doing this repeatedly, it was possible to determine a curve relating tankage requirement and tanker availability. Two things were used to determine this curve. First, the available information, secondly, the random distribution type of occurrence of certain events. On the basis of these, it was possible to decide whether or not a certain tankage should be kept or sold.

Ph. Dreyfus: A tanker fleet capacity would be defined once and for all, whereas the problem here is to establish a programme for a fleet of ships. This programme will have to be available for months or years, so it cannot be established once and for all, because there will be some random data which will disturb the planning as time elapses. One could never, of course, keep up with the programme, so there must be some kind of dynamic scheduling available. Do you know of any application in this field?

Dr J. T. Ahlin: One approach has used game theory methods. Several examples can be mentioned which, for example, give methods for determining the requirements of a tanker or tank car fleet. However, the actual scheduling of a tanker fleet on a dynamic basis is usually done by simulation techniques. Significant results have been obtained by these methods, and to date this appears to be the most satisfactory approach.

Dr G. G. Hall: Dr Barnett has described the main topics in theoretical chemical research which are of interest to oilmen, but I would like to emphasize the importance of one of these, namely calculations of the most fundamental sort, which start from the Schrödinger equation and assume very little else. One aspect of this, which will be of considerable interest, is the calculation of the structure and properties of very short-lived intermediates. There are various radicals and ions which live for so short a time that they cannot be studied experimentally. Computers will be most useful in enabling us for the first time to study these things.

In the U.S.A. a great deal of this fundamental research is done by the universities on machines owned or rented by oil companies. These are made available to the universities freely at night, so that there is no conflict with their ordinary use, and it is no exaggeration to say that the fate of a department doing theoretical chemistry in the U.S.A. depends exactly on how much of this co-operation it can get. Those people who have some control over the machines should consider this very carefully.

Dr M. P. Barnett: Computers have been applied in the U.S.A. to all the theoretical chemical topics mentioned in the paper, and these topics are all of some importance to the petroleum industry. It would be of interest if some comment could be made on theoretical chemistry applications in European petroleum laboratories.

Ph. Dreyfus: Our computer has been used to tackle two of the problems mentioned. One is the calculation of the atomic structure factor resulting from X-ray crystallographic analysis, and the other is the determination of electron energy levels of organic and complex molecules. These two problems have been treated in France by the Gamma computer. Neither of these cases was for the oil industry. The electron energy level was for a Cancer Research Institute, and the other was for pure crystallographic laboratory work.

Dr R. J. Lunbeck: The question was raised as to whether the Amsterdam electronic computer was used for fundamental research, in particular for quantum mechanics, and if so whether outsiders could make use of it.

The Ferranti Mark I* computer was installed in the Amsterdam laboratories of the Royal Dutch/Shell Group about two years ago, and since then has been intensively used for a great variety of problems, among which several were of a fundamental nature, *e.g.* quantum mechanical calculations.

The number of applications is such that only very occasional work can be done on behalf of outsiders.

W. H. Thomas: Is there any experience of the use of computers to avoid the bunching of tankers?

C. M. Berners-Lee: My company has not undertaken any applications of Monte Carlo methods to tanker queueing. However, a most successful investigation of a more familiar queueing problem was undertaken on one of our machines, using a Monte Carlo method. The problem related to the regularity of a bus service. In the computer model, buses were sent out at regular intervals and subjected to random delays, and the effect of a number of different possible operating procedures on the regularity of the service was studied. Such procedures included allowing buses to overtake, relaxing the rules about buses not being permitted to pass certain points ahead of schedule, and enlarging garages at either end of the route in order to allow de-randomizing at the termini.

J. B. Bretscher: So far, the problems which have been discussed have involved the solution of mathematical functions of a polynominal or determinant type. I would like to know whether a computer has been used in the solution of more complex types of functions, such as the differential equations which occur in reservoir engineering, some of which are fairly complicated.

Dr M. P. Barnett: One project which immediately comes to mind is the use, in New York by Dr Kogbetliontz, of the 701 in the solution of the partial differential equations describing reservoir depletion.

Dr J. T. Ahlin: Some of the most interesting areas of computer application are those concerned with solving partial differential equations. It is felt that the solving of ordinary differential equations, even of a non-linear type, has been fairly well examined, and a great many worthwhile results have been forthcoming. Several of the petroleum companies, of which two in particular come to mind, have been spending many years in actually studying problems of reservoir mechanics, and it turns out that the three basic equations with which one deals are partial differential equations; namely, the equations of state, conservation of mass, and the Darcy equation. These have been handled and solved. Techniques have also been studied and solutions found for handling moving boundaries, which are of considerable interest in reservoir studies. One group studied recently, on the 704, a reservoir problem which had actually been determined would take some 200 hours on the medium-scale computer. This was actually solved on the 704 in 15 minutes. Since this was the study of fluid injection, the group was interested in determining the effects of injection at various wells in a field. It represented substantial time saving, even with the large machine, and it certainly would have been inconceivable even to think about it by any other method. These equations which arise do not lend themselves to analytical solution in any form known. In some cases successful solutions have been obtained. However, it cannot be stated that all types of partial differential equations which are known to represent physical systems, particularly in reservoirs, have been solved as yet. There is still a lot of work to be done.

P. Mayers: Reverting to the question on the bunching of tankers, we have done some studies on the provision of sufficient berthing facilities to avoid uneconomic ship waiting time by roughly similar methods to those which Dr Ahlin described. The Monte Carlo technique was employed, using the distribution curves for the arrival of tankers over a limited period, shut-down of various berths for dredging, specifications that certain types of ship must go to a certain berth, and similar things by which one can arrive at the necessary jetty facilities to avoid, or to reduce to a minimum, the ship waiting time. The actual waiting time can also be predicted for various arrival patterns and different jetty facilities.

Dr M. P. Barnett: In regard to partial differential equations in petroleum work, a few more examples come to mind. In one method of oil prospecting, electrical equipment which measures the resistivity of the peripheral soil and rock is lowered down a shaft. For the calibration of certain equipment of this type calculations were performed on the Whirlwind computer at M.I.T., which involved the solution of partial differential equations of a rather unpleasant type.

Another example of the solution of partial differential equations is in connexion with combustion theory, predicting, for example, flammability limits of fuel mixtures.

A further application relates to a project in which oil is injected underground at one point to produce a pressure front which will drive oil to the surface. In connexion with this, a computer is being programmed to solve the relevant partial differential equations.

W. H. Thomas: I would like to thank the authors of the papers for a very clear exposition of their subject matter and also to express our combined admiration for the way they have answered the difficult questions which have been put to them.

The occasion should not pass without expressing our tribute to Dr Ahlin for coming all the way from the U.S.A. to talk to us. The U.K. is still on the threshold of the use of this type of equipment, and American experience has already proved extremely valuable.

Most of the data given in the ASTM/IP Petroleum Measurement Table were calculated by ordinary hand machines. These tables have already been of tremendous advantage to the oil industry, but they could have been calculated much more quickly by a digital computer and with far less probability of error. For example, the rounding-off of values has not been always consistent, and the result is that certain numerical inconsistencies have been noted. There is a tremendous amount to be gained by putting refinery planning on a proper mathematical basis. Such planning at present is largely the result of past experience and intelligent guesswork, although it must be conceded that very few major mistakes are made. It is not known, however, whether our refineries are run economically and whether the maximum profit is obtained. We have had examples of the programming of specific plants, but with the whole refinery there are a great many factors to be considered—the input of a refinery, the qualities of the various finished products, the number of finished products, all these factors being allied to the plants available, with but little data on their maximum throughputs. This is a problem of programming which will occupy a number of mathematicians for a year or so. When it has been solved, what is the next stage and what is the computer going to do next? Will it just go on working on the same tasks, or will the mathematicians proceed to resolve all the other hitherto insoluble refinery problems?

The meeting then closed with a unanimous vote of thanks to the authors of the papers.

PRE-FLAME REACTIONS IN DIESEL ENGINES

PART IV. THE EFFECT OF COMPRESSION RATIO*

By F. H. GARNER,† O.B.E. (Past-President), FRANK MORTON,‡ (Vice-President), J. B. SAUNBY † (Student Member), and G. H. GRIGG † (Student Member)

SUMMARY

In previous publications[1, 2] the results of analysing samples drawn from the combustion chamber of a Crossley engine, fitted with a Comet Mark II cylinder head, have been reported. These samples were analysed for aldehydes and peroxides. The detection of pre-flames using a photomultiplier unit was also described.

The effect of other variables, primarily compression ratio, has been investigated using a CFR diesel testing unit. As in the previous work, pre-flames of varying intensity have been observed both before and after the injection of fuel, mostly at high compression ratios. The nature of the delay period and the effect of temperature and pressure on ignition lag have been examined in an attempt to explain the anomalies present in the family of curves of ignition delay *v.* compression ratio.

INTRODUCTION

ALTHOUGH more interest is currently being shown in the mechanism of combustion in the diesel engine, the amount of information so far available compares unfavourably with that for the petrol engine. This is probably due in no small manner to the heterogeneous nature of the reaction in the diesel engine which makes the investigation more difficult.

The reactions occurring during combustion can be examined by two different methods: (1) analysis of the reactants and products at varying stages during the reaction, and (2) a thermodynamic approach based on pressure and temperature measurements. In the former, samples of gas are withdrawn from the reaction chamber and analysed by chemical means. This method has been used for diesel combustion by several investigators,[1-3] but limitations are imposed by the time necessary for the collection of the sample and the resulting decomposition of unstable intermediates. The detection of small quantities of complicated organo-peroxides is also difficult. Other means of analysis used are spectrographic methods. Although this has proved successful in the case of combustion in the petrol engine, as is evidenced by the work of several investigators,[4-6] it is not suitable for the study of diesel combustion. This has been shown by Lyn,[7] who in his study of the combustion process by infra-red emission spectroscopy found the normal hydrocarbon flame spectra obscured by the continuous radiation from carbon particles.

Pressure and temperature measurements in both motoring and firing engines have been used to give some insight into the pre-combustion reactions, and this method may offer a more rigorous solution to the problem. Rifkin *et al* [8] and, more recently, Olson, Wentworth, and Daniel,[9] have made a thermodynamic analysis both of the pressure developed and the energy released during the pre-flame period. This work has confirmed the fact that the ignition of hydrocarbons in the diesel engine takes place by a two-stage process. Most of the work on the effect of temperature and pressure on the two induction periods, which is applicable to the conditions encountered in the diesel engine, has been carried out in rapid compression machines. The original work was that of Tizard and Pye,[10] later continued by Jost,[11] Scheuermeyer and Steigerwald,[12] and by Rögener.[13] Recent work by Livengood and Wu [14] indicates that the results obtained using rapid compression machines can be compared with those obtained with both motoring and firing engines.

A comparison is made in the present work, where the effect of temperature and pressure on the ignition lag in the engine is examined by varying the compression ratio and observing the effect on the point of flame arrival. The results show good agreement with those obtained by Scheuermeyer and Steigerwald using a rapid compression machine.

EQUIPMENT

The engine is a standard CFR–ASTM diesel-testing unit which incorporates a precombustion chamber cylinder head. The recommended standard operating conditions were maintained as given in Table I.

TABLE I

Speed	900 rev/min ± 9 rev/min
Injection timing	Variable
Injector opening pressure	1500 p.s.i. ± 50 p.s.i.
Fuel rate	13·0 ml/min ± 0·2 ml/min
Lubricating oil	SAE 30
Oil pressure	25–30 p.s.i.
Oil temperature	135° F ± 15° F
Coolant temperature	212° F ± 3° F
Intake air temperature	150° F ± 2° F

The instrumentation of the engine was modified to enable the point of injection and ignition to be measured. Standard Sunbury indicating equipment

* MS received 23 October 1956.

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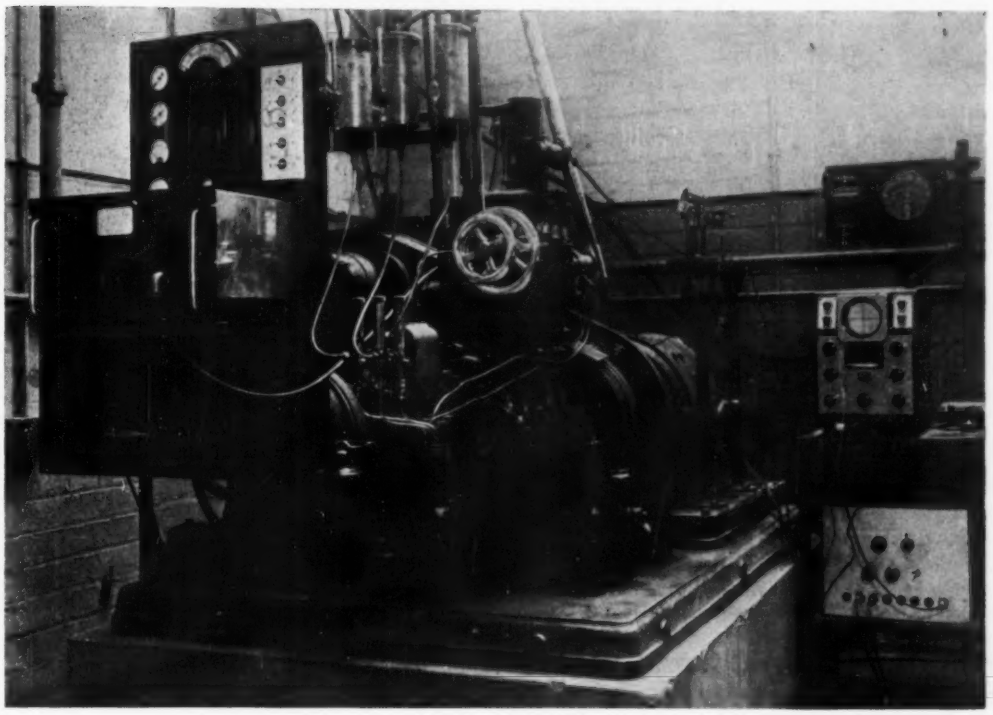

FIG 1

GENERAL LAYOUT OF ENGINE AND EQUIPMENT

was used for measurement of the crank angle position of injection, the indicators being connected to a Cossor double-beam oscilloscope. A time sweep and degree marker unit was coupled to the engine crankshaft, and this triggered the time base of the oscilloscope, supplying the signal for the horizontal degree scale on one of the two beams. Point of injection was measured by an electro-magnetic pick-up fitted to the injector.

The point of ignition was determined by using a photomultiplier unit, RCA 931, as described previously.[1] An adaptor to carry a silica window was made so that the window fitted in the same position as the metallic disk used in the bouncing pin method for recording the point of combustion. This meant that the absolute compression ratio–handwheel setting relationship remained unaltered. This adaptor is shown in position in the cross-section of the cylinder head, Fig 2. Initially, trouble was again experienced with the washers supporting the window at high compression ratio or when heavy knock occurred, but this was finally overcome by using metal reinforced " halite " washers.

A constant voltage power supply to the photomultiplier was obtained from a power pack giving 1200 V stabilized d.c. The output from the last stage of the photomultiplier was passed through a 750-Ω resistor to earth and the output across the resistor was led to the oscilloscope. When carbon formation occurred on the window, the internal amplification of the oscilloscope was usually sufficient to give a definite point of ignition.

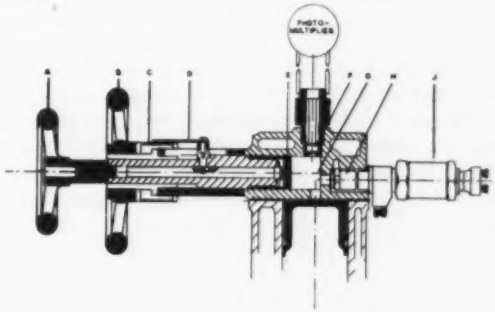

FIG 2

DETAIL OF CYLINDER HEAD

A—Locking wheel
B—Compression ratio adjusting wheel
C—Micrometer scale sleeve
D—Micrometer scale arm
E—Expansion plug
F—Silica window
G—Combustion chamber
H—Injector
J—Injection indicator

FUELS

Two fuels, D1, a high-cetane, paraffinic secondary reference fuel, cetane number 70, and D6, a low-cetane naphthenic gas oil, cetane number 32, were used. Inspection data for these fuels have been reported previously.[2]

RESULTS

Preliminary runs showed that although the CFR engine is designed to operate at an injection setting of 13° b.t.d.c., a large range of settings earlier than this could be used, extending from 30° b.t.d.c. up to 5° b.t.d.c. It was also found possible to vary the fuel rate over quite a large range.

The first series of runs was carried out at the standard fuel rate of 13·0 ml/min for both fuels, the compression ratio being varied from 11·0 to nearly 30·0 over the range of injection settings mentioned previously. It was decided to use a constant volume fuel rate so as to keep as close to standard operating conditions as possible but even so this only made a difference of 1200 B.t.u. or 4 per cent in the heat input for the two fuels.

The results for the two fuels are shown graphically in Figs 3 and 4, where ignition delay is plotted against compression ratio with injection timing as parameter.

Pre-flames of varying intensity were found with both fuels, but only at high compression ratios. With fuel D1 at the early injection settings 30° and 25° b.t.d.c., pre-flames were present at compression ratios of 21·6 and 29·2, but absent at the intermediate value of 24·5. At this setting, a pre-flame appeared to be merging with the main flame. Photographic records of these effects are shown in Fig 5. In these figures the upper trace is the degree scale in which the highest vertical stroke marks the position of t.d.c. approached from left to right on the compression stroke, the lower trace is the flame intensity curve, the lowest point corresponding to maximum intensity. Fig 5 (*a*) shows the small pre-flame present at a compression ratio of 21·6, Fig 5 (*b*) the effect at 24·5, and Fig 5 (*c*) the distinct large pre-flame present at 29·2.

With fuel D6, pre-flames were again observed but only at the higher compression ratios. At an injection setting of 20° b.t.d.c. a small pre-flame occurred at a compression ratio of 29·2 and at 24·5 the pre-flame was again merging with the main flame as for fuel D1. Small pre-flames were observed at all injection settings at a compression ratio of 29·2. As the compression ratio was lowered at an injection timing of 20° b.t.d.c., knocking started at 21·6 and got progressively more severe until at a compression ratio of 14 very heavy knock limited the operation of the engine. It was observed that between these two values the engine occasionally ran without knocking

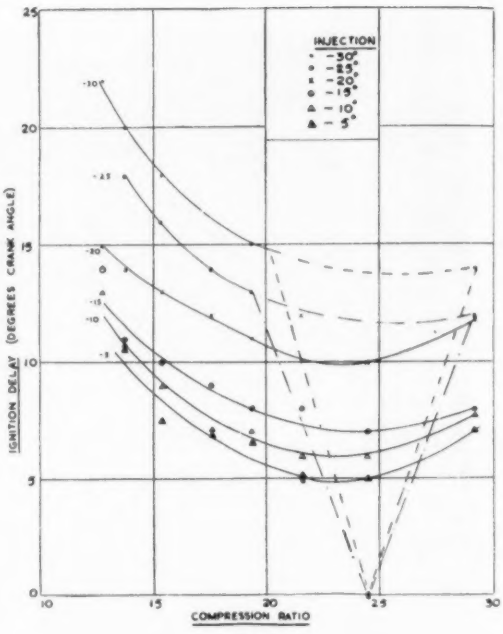

FIG 3
FUEL D1
Rate, 13 ml/min

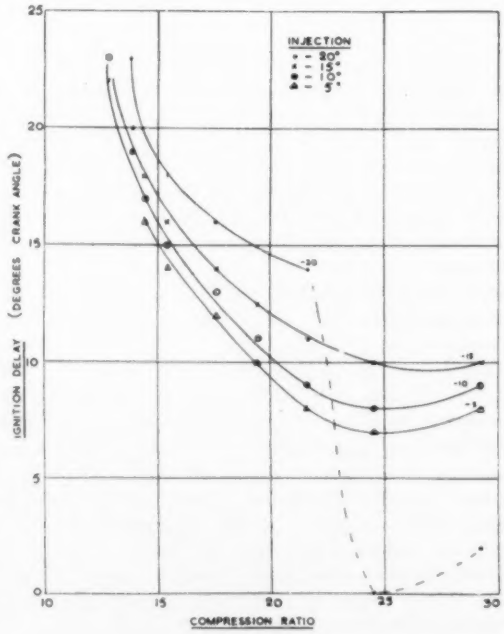

FIG 4
FUEL D6
Rate, 13 ml/min

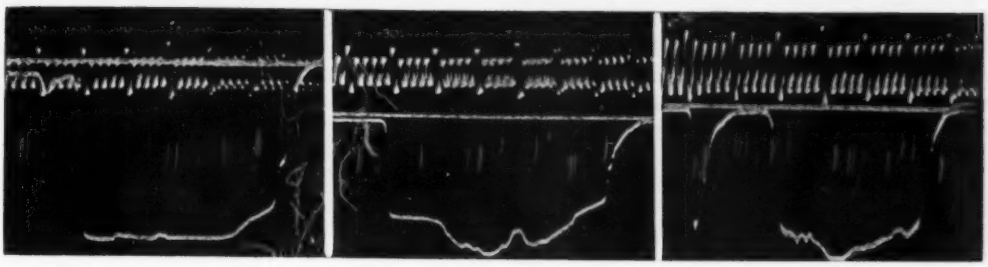

FIG 5

(*a*) C.R. 21·6 (*b*) C.R. 24·5 (*c*) C.R. 29·2

for several revolutions. When this occurred, ignition invariably took place at about 10° b.t.d.c.

Following these two series of runs, it was thought that the effects noticed at the early injection timings and high compression ratio, *i.e.* zero ignition delay, were due to fuel being carried over from the previous power stroke either as droplets or on the walls of the

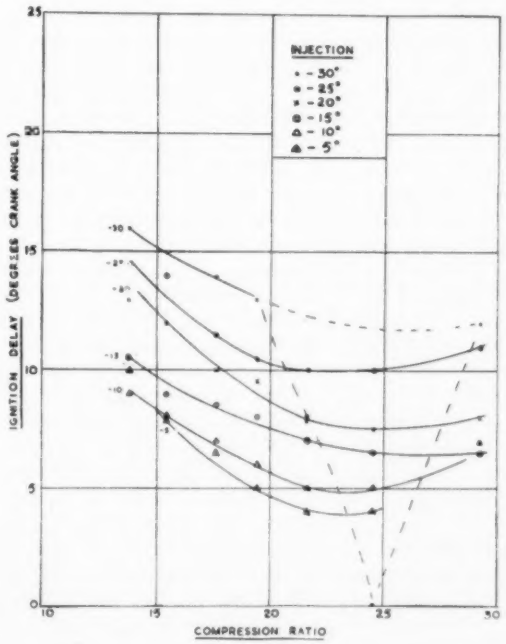

FIG 6

FUEL D1

Rate, 11 ml/min

engine or as intermediates, and igniting on the next compression stroke as soon as the temperature and pressure were sufficiently high. The presence of fuel carried over was supported by the fact that very black exhaust smoke was observed, showing incomplete combustion. It was therefore decided to operate at lower fuel rates to see the effect on delay at early injection settings. The results for a fuel rate of 11 ml/min are shown in Fig 6, and it can be seen that combustion occurs normally at an injection setting of 25° b.t.d.c., but at 30° b.t.d.c. results similar to those for a fuel rate of 13 ml/min are again observed. At this setting, similar signs of incomplete use of the fuel were observed. Reducing the fuel rate to 9 ml/min gave the results shown in Fig 7, and again the small pre-flame at a compression ratio of 21·6, merging of pre-flame and main flame at 24·5, and a separate pre-flame at 29·2 was observed. Again, incomplete use of the fuel was observed at these higher compression ratios, but it was not possible to reduce the fuel rate further because of the limited range over which the engine would then operate and because of a possibility of changes in the characteristics of the fuel pump and injection equipment.

The general trend is a decrease in the delay period as the compression ratio is increased until some critical point is reached, after which the delay period again begins to lengthen : this applies for both D1 and D2 and for all three fuel rates with D1. For fuel D1 this critical compression ratio is 23 : 1 and for D6 25 : 1. For D1 the early injection settings 30° and 25° b.t.d.c. show a break at 24·5, and D6 shows a similar sort of break at an injection setting of 20° b.t.d.c. and the same compression ratio, 24·5.

DISCUSSION OF RESULTS

The ignition delay under varying conditions can be considered as made up of a physical and a chemical delay. Considering physical delay first, following the injection of the fuel into the precombustion chamber the first physical step is evaporation from the fuel droplets. This appears to be the most important factor in the physical delay period. The rate of evaporation is influenced not only by the properties of the fuel but also by the temperature of the air in the precombustion chamber, the velocity of the droplets, the air density in the chamber, the path that the droplet can travel without impingement, and also the movement of the air (" swirl ") within the chamber. Although it has been assumed in this investigation that

the combustion process is unaffected by the method used to vary the compression ratio, in the CFR, with its unconventional precombustion chamber, the effect may be appreciable. The effect of increasing the compression ratio is to increase the rate of vaporization of the droplet owing to the rise in temperature of the compressed air and, although the greater gas density may lead to a lower droplet velocity, the friction on the droplet will be greater. The amount of swirl is dependent primarily on crank angle position of injection and will not alter appreciably. At the higher

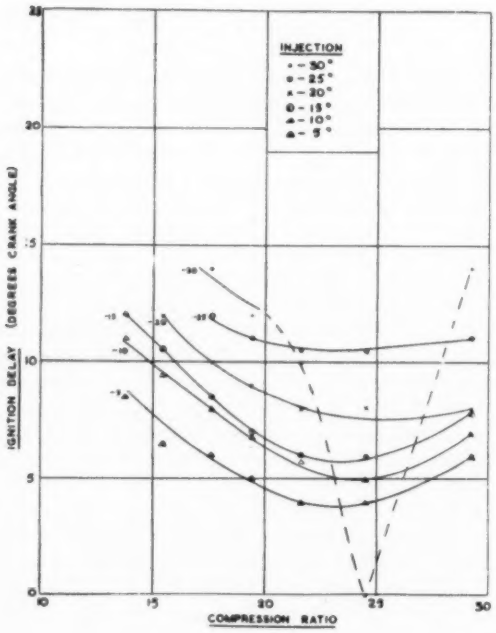

FIG 7
FUEL D1
Rate, 9 ml/min

compression ratios, when the length of the precombustion chamber is little more than 0·5 inches, the effect of impingement of the fuel spray on the opposite wall may well be appreciable; Vulliamy [15] found a distinct improvement in the characteristics of a precombustion chamber engine by elongating the chamber. The overall effect of increasing the compression ratio will be to shorten the physical delay period until the effects of impingement come into play. If physical delay is controlling, then a plot of ignition *v.* compression ratio would be expected to show a minimum at some high compression ratio, and this holds for Figs 3, 4, 6, and 7; if this were due solely to the physical factors outlined above, then the point at which the minimum occurs should be the same for each fuel. As this is not the case, it was concluded that the physical delay is not controlling.

After partial evaporation of fuel drops the next step is the reaction between fuel vapour and oxygen at the fuel–air boundaries, the nature of this reaction depending to a large extent on the temperature and pressure obtaining. It has been suggested [16] that as soon as these reactions have proceeded sufficiently and the local temperature is high enough, the fuel vapour phase begins to crack and may precipitate materials with a high carbon percentage, which by virtue of localized conditions become heated to incandescence, the precipitated carbon being either consumed during the combustion cycle or emerging as soot.

The reaction between fuel vapour and oxygen may take place by several different routes, since, as shown by Fig 5, the pre-flame reactions emit light of different intensity at varying times before the main flame appears. It seems likely that at the early injection settings 25° and 30° b.t.d.c. (D1) and 20° b.t.d.c. (D6), fuel is being carried over from the previous power stroke, when a weak but almost homogeneous fuel–air mixture would be present in the combustion chamber during the compression stroke. The conditions during this part of the cycle (before the injection of fuel) are then similar to those encountered by Rögener,[13] who investigated the effect of temperature and pressure on the induction period, using a rapid compression machine. The adiabatic compression temperatures attained in Rögener's experiments range from 400° to 500° C, and the pressure from 5 to 40 atm, while in the present work at an injection setting of 30° b.t.d.c., a compression ratio of 20 corresponds to a temperature of 454° C and a pressure of 17·4 atm, and a compression ratio of 30 to a temperature of 492° C and a pressure of 21·1 atm. It seems justifiable to compare our CFR results with those of Rögener. His experiments showed that the ignition of hydrocarbon–air mixtures is by a two-stage process with two separate induction periods τ_1 and τ_2, and these regions culminate in cool flames or hot ignition respectively, when the temperature and pressure exceed the critical limits; the temperature and pressure of the system is, of course, raised as the compression ratio is increased. The effect of temperature and pressure on the induction period is now therefore considered, bearing in mind the presence of fuel in the combustion chamber from the previous power stroke.

Andreev,[17] in agreement with Aivazov and Neumann,[18] found that τ_1 decreased continuously with increasing temperature, while τ_2, which is very small compared with τ_1, increased with temperature. Also, information obtained by Neumann and Tutakin [19] showed that τ_2 steadily decreased as the pressure of a given mixture was increased, and this was also confirmed by Kane.[20] The overall picture of the induction period is that, with increasing temperature, τ_1 decreases and τ_2 increases, whilst with increasing pressure τ_1 and τ_2 decrease. It should be noted, however, that the decrease of τ_1 with temperature is

more rapid than the corresponding increase of τ_2 and that τ_2 decreases with pressure more rapidly than τ_1.

The results from the CFR engine can now be examined in the light of these remarks. Considering the curves for injection timings of 30° and 25° b.t.d.c. in Fig 3 at compression ratios 21·6, 24·5, and 29·2, ignition occurs as shown in Fig 5. In Fig 5 (*a*) a small pre-flame occurs with a short time interval before the main flame, whereas in Fig 5 (*b*) the pre-flame and main flame merge to give an apparent zero delay period. When the compression ratio is increased to 29·2, a discreet pre-flame again appears (Fig 5 (*c*)), of

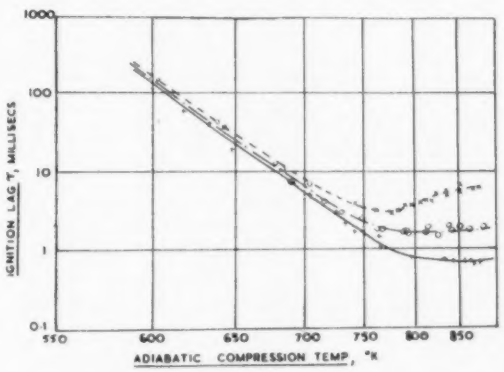

FIG 8

DATA OF SCHEUERMEYER AND STEIGERWALD FOR *n*-HEPTANE

greater intensity than at the compression ratio of 21·6 and with a greater time interval between it and the main flame. From the foregoing discussion on the effect of temperature and pressure on the delay period, the following explanation is suggested. In the case of a compression ratio of 21·6 as shown in Fig 5 (*a*), τ_1 is controlling. As the temperature is increased τ_1 decreases and τ_2 increases up to the point where $\tau_1 + \tau_2$ is a minimum, and in this case pre-flame and main flame merge, as shown in Fig 5 (*b*). As the temperature is further increased τ_2 increases to give a discreet pre-flame, as shown in Fig 5 (*c*).

Returning to the normal family of curves for ignition lag *v.* compression ratio, the general trend of decreasing ignition lag with increasing compression ratio with a minimum value is similar to the effect observed by Scheuermeyer and Steigerwald [12] on *n*-heptane, as shown in Fig 8. At low temperatures each curve conforms to a straight line τ decreasing by a factor $e^{\text{CONST}/T}$ indicating that τ_1 is predominant. At higher temperatures the ignition lag tends to increase, conforming to the trend of τ_2, which increases with increasing temperature. A better comparison with the CFR results can be made if the theoretical adiabatic compression temperature at the point of ignition, *i.e.* the end of the delay period, is plotted against ignition lag. This is shown for a typical case in Fig 9, the injection being 15° b.t.d.c. with a fuel rate

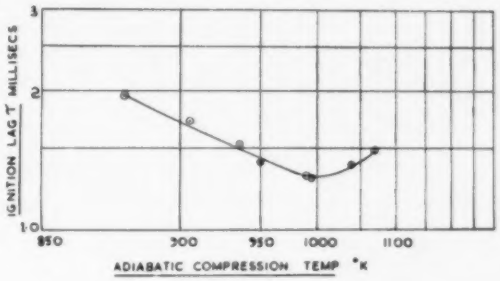

FIG 9

FUEL D1

Rate, 13 ml/min
Injection, 15° b.t.d.c.

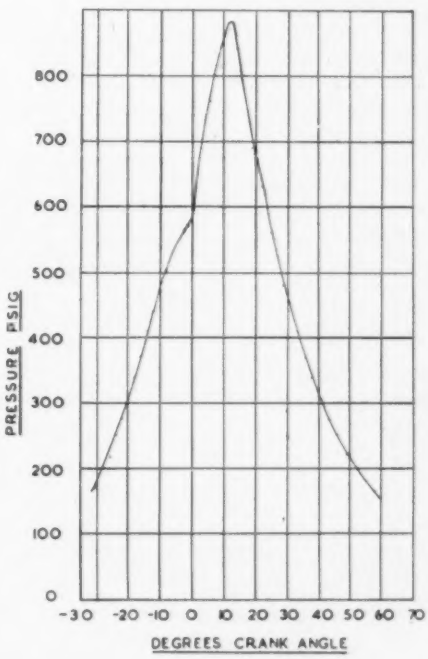

FIG 10

FUEL D1

Fuel rate, 26 ml/min
Injection, −10°
Ignition, −1°

13 ml/min of D1. In this diagram it can be seen that at the lower temperatures the curve again conforms to a straight line. At higher temperatures the ignition lag tends to increase, conforming to the trend of τ_2.

The temperatures used in constructing Fig 9 are

those calculated theoretically, assuming the compression up to the point of ignition to be adiabatic. The temperature is then calculated from the ratio of the specific heats for the gas mixture in the cylinder, the swept and total volume, and the volume of air admitted per cycle. The value of γ, the ratio of the specific heats used in the equation $PV^{\gamma} = \text{const.}$ for adiabatic compression, is taken from information reported by Hershey *et al.*[21]

Although the absolute values obtained for the temperature are open to error, the relative values will be consistent. Earlier work on the Crossley engine[22] suggested that this method of calculating cylinder temperatures prior to ignition was at least as accurate as calculating these temperatures from pressure diagrams constructed using an absolute pressure calibrating unit. This unit was unable to detect pressure rises in the pre-flame region, due primarily to the cyclic variations which occur in diesel engines, and the pressure–time curve was smooth up to the point of ignition for all injection timings. A typical curve is shown in Fig 10.

Future work is aimed at making a more rigorous examination of the effect of temperature and pressure on the pre-flame period by direct temperature measurements. Simultaneous pressure and temperature measurements will be made using a rate of change of pressure indicator of the diaphragm type in conjunction with an electronic integrator to give absolute pressure–time records and a modified sodium reversal line technique for temperature measurement.

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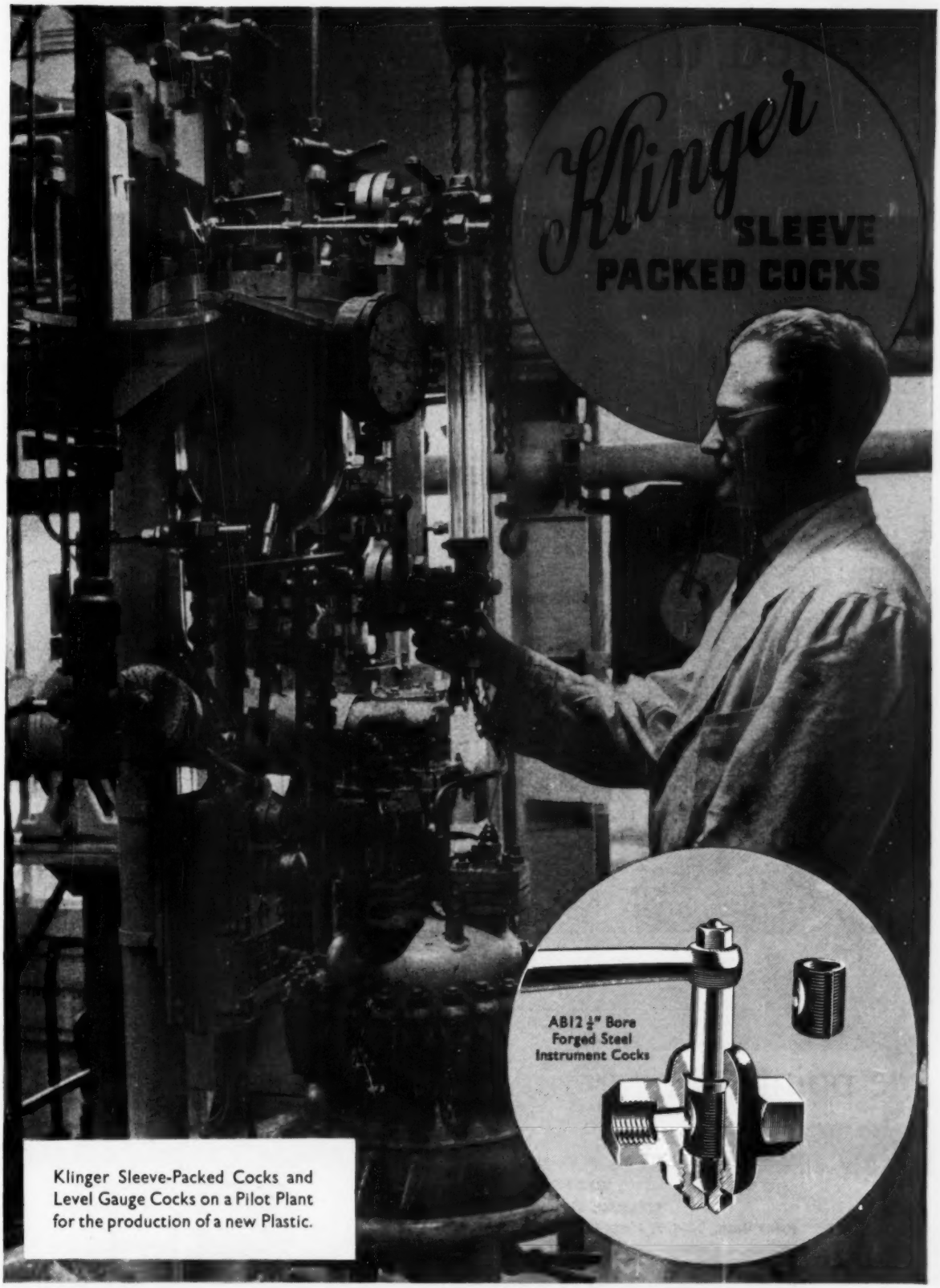

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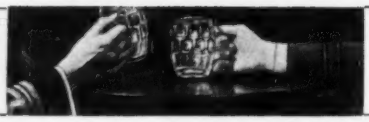

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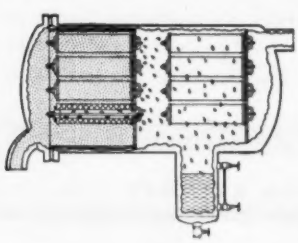

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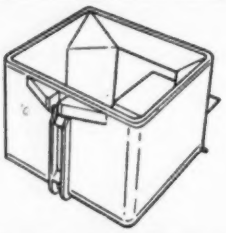

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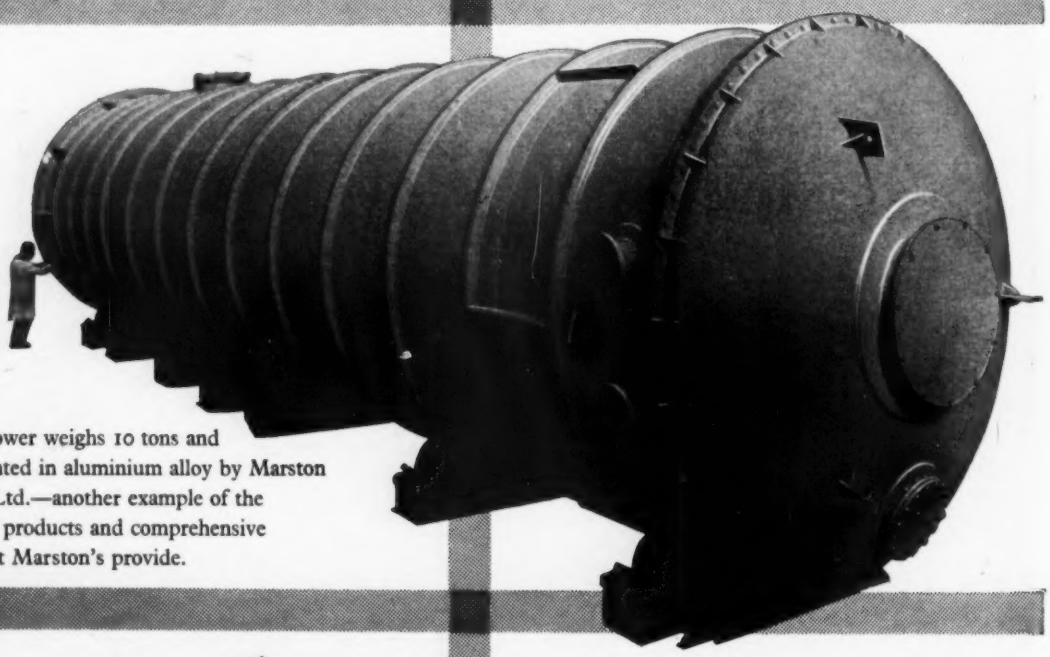

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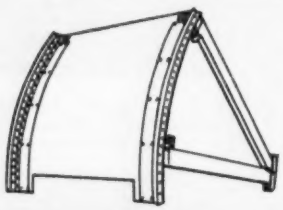

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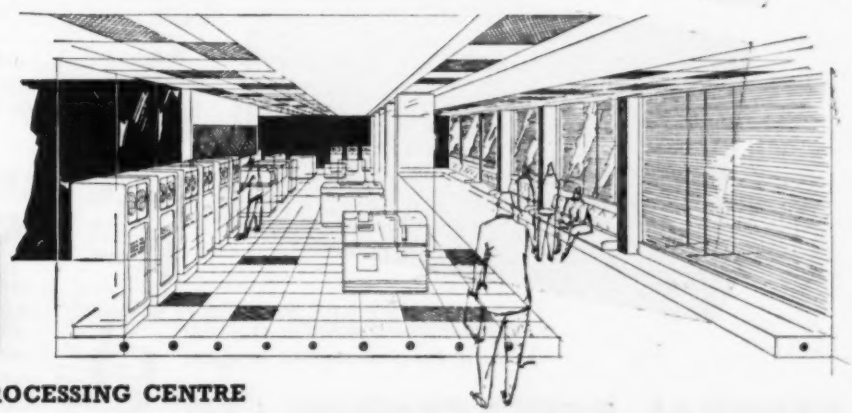

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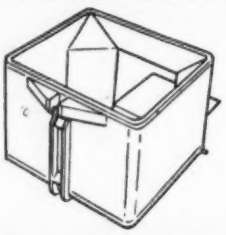

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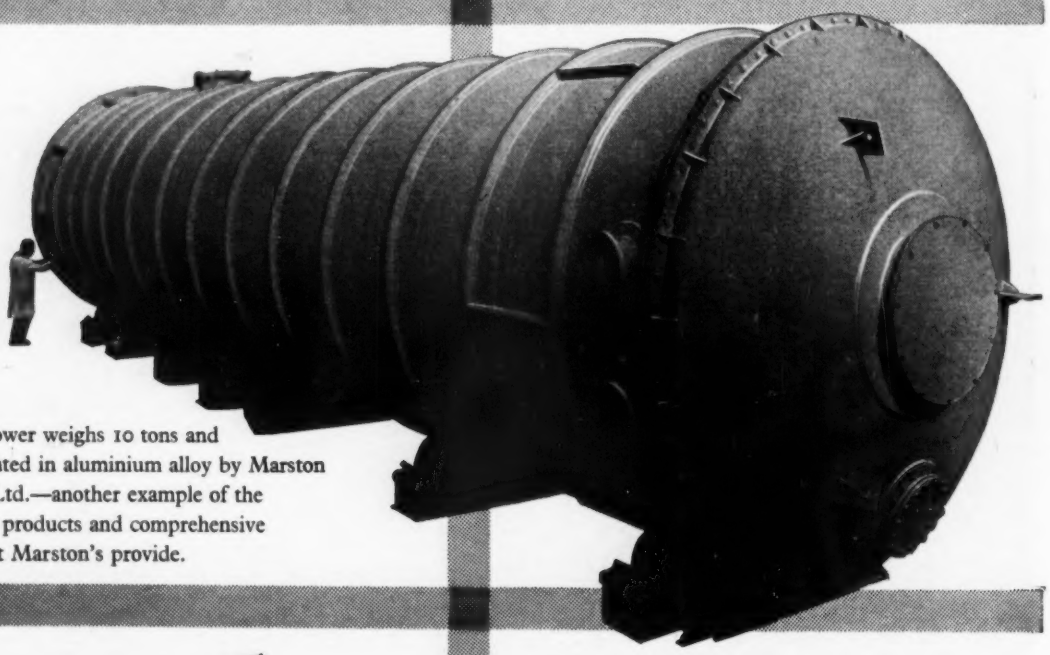

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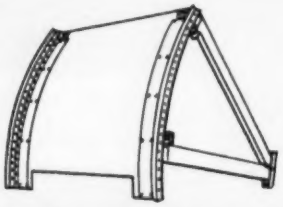

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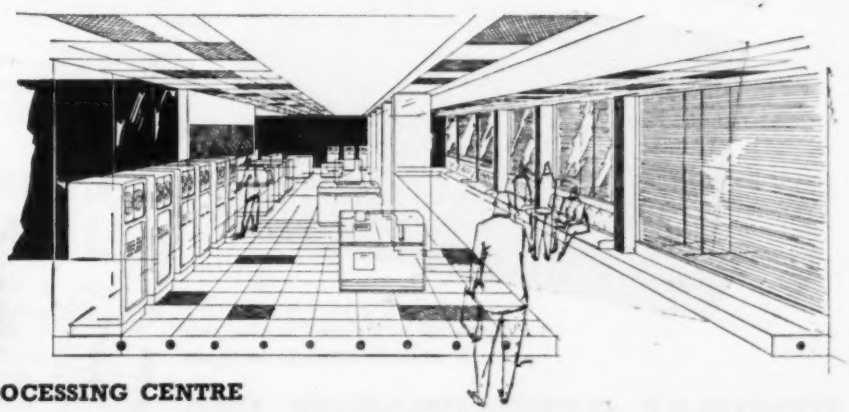

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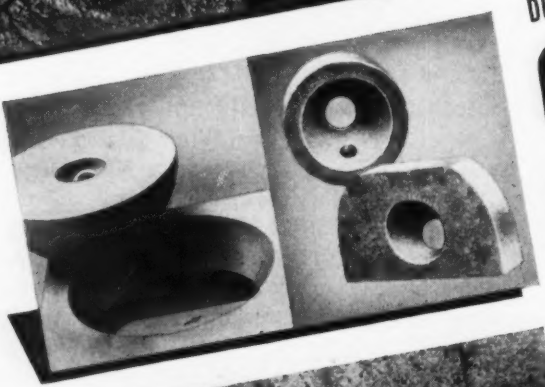

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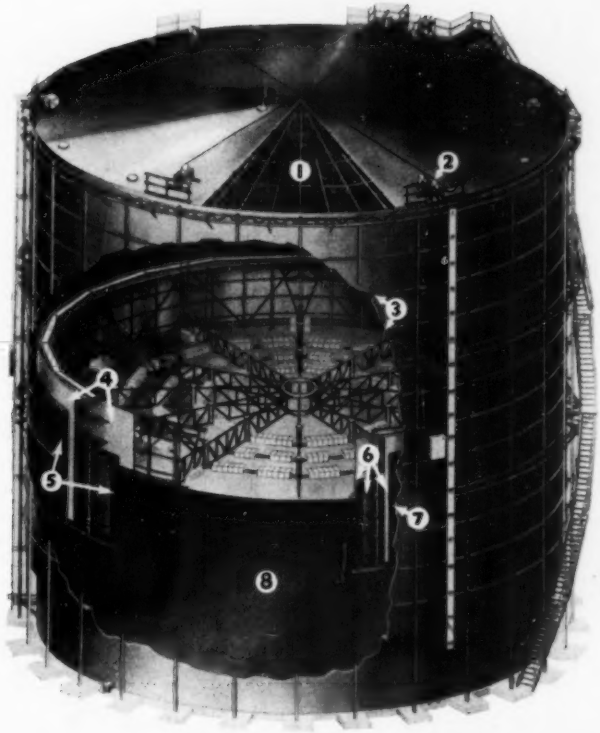

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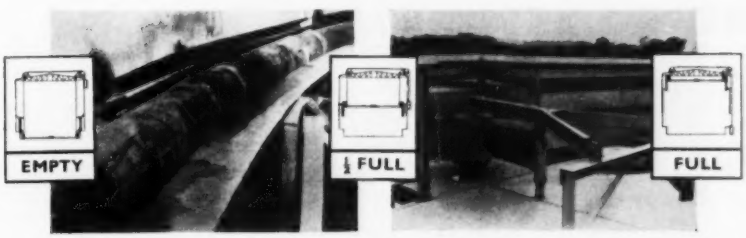

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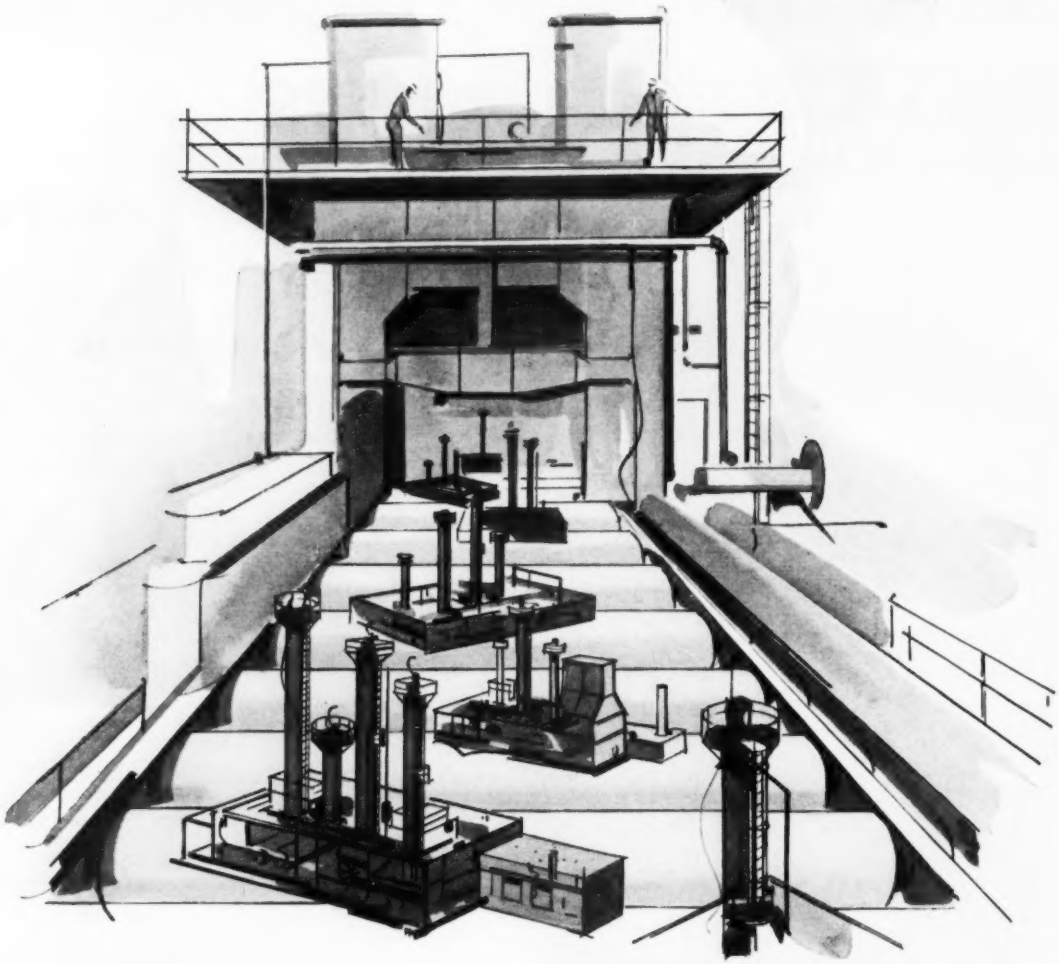
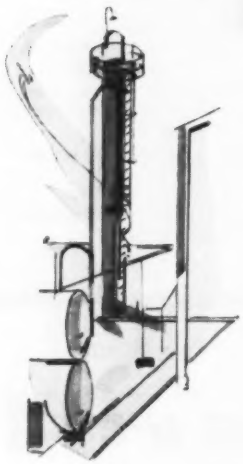


There's no production line for plant construction



There's nothing routine about this business of building petroleum refineries, chemical plants, and petrochemical plants. Every construction project is a different problem, a fresh challenge, an opportunity for new accomplishments. That's why we've assembled here at Procon an engineering and construction staff with the broad experience, the technical know-how, and the creative enthusiasm to meet and master any construction problem to your better-than-ordinary satisfaction. If you are in a building mood, Procon can help you!

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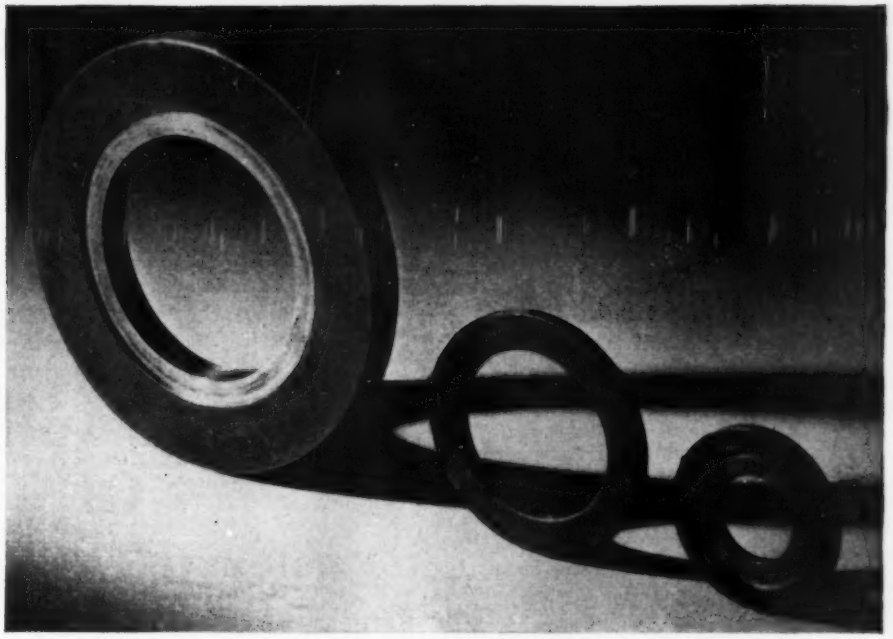
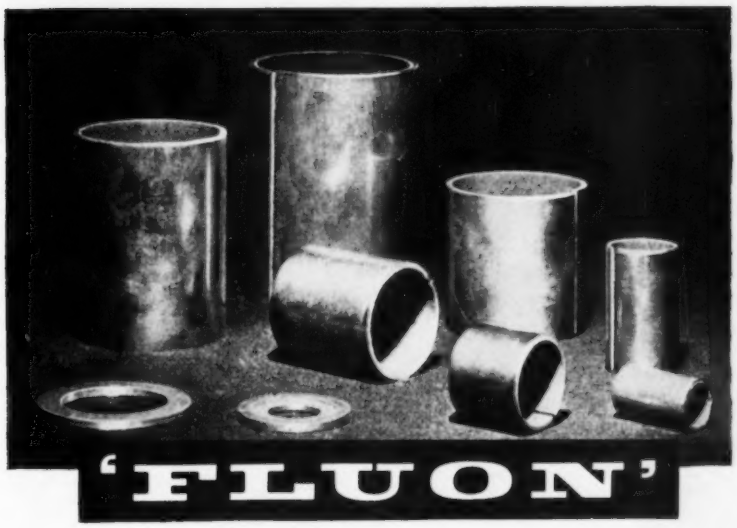


The thrust washers and bearings impregnated with 'Fluon' shown in the two pictures, are manufactured by The Glacier Metal Co. Ltd., London.

'FLUON' impregnated bearings cut out lubrication



'Fluon' is the registered trade mark for the polytetrafluoroethylene manufactured by I.C.I.

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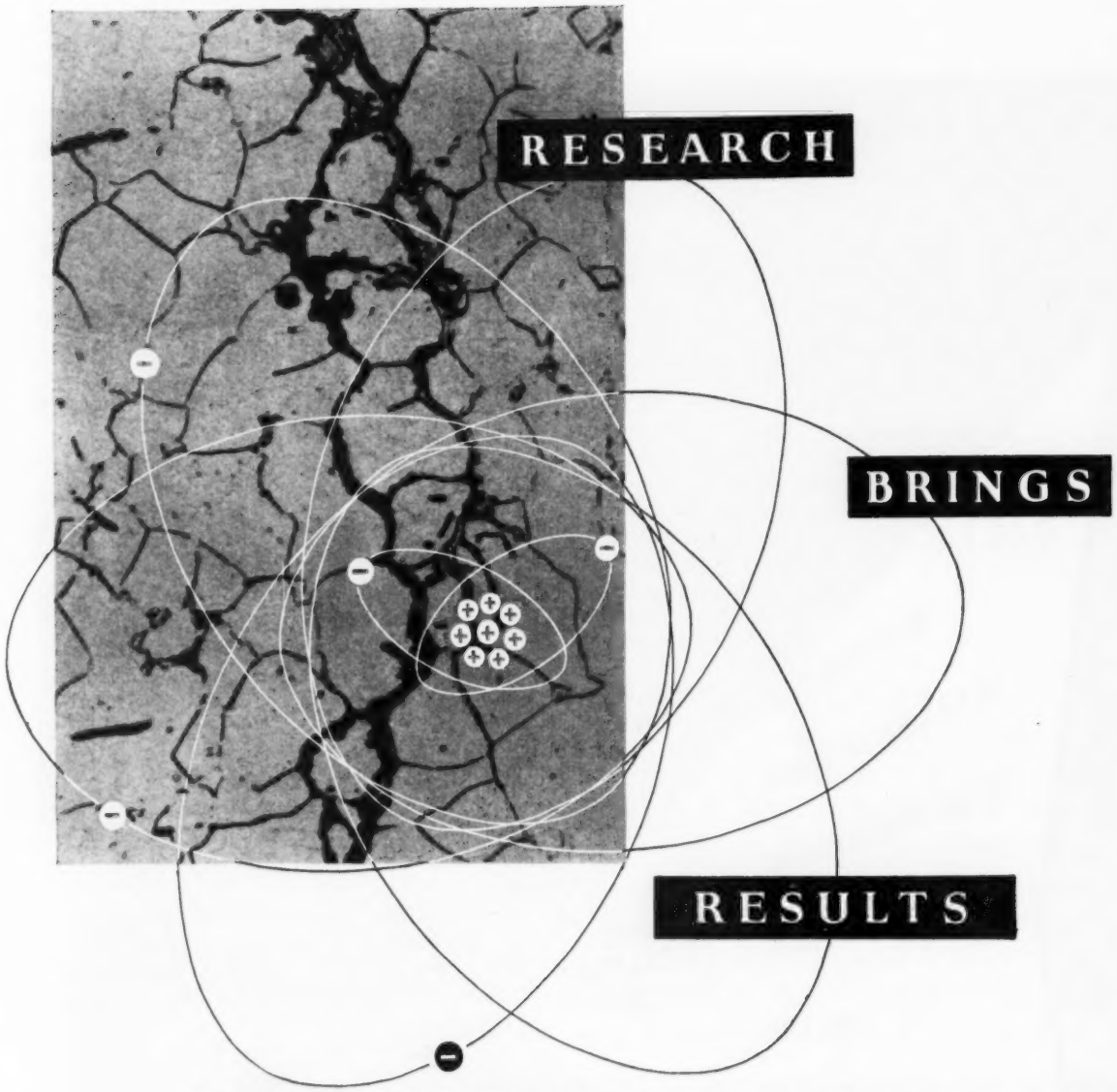

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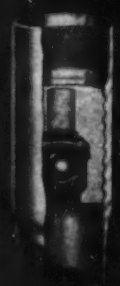

This is the time-tested Baker Cement Float Collar (Product No. 101 M&F) usually positioned just above the shoe joint to provide a "stop" for the cementing plug. Used in combination with any type of Baker Cement Float Shoe, Guide Shoe, or the "Whirler" Shoe to meet the customer's need.

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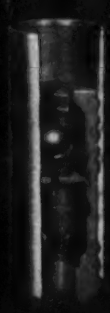

This is the new Baker FLEXIFLOW Fill-Up Shoe (Product No. 168) Permits casing to fill from the bottom through a hole in a flexible diaphragm that opens up to relieve dangerous high pressure surges and closes down to control casing fill. Cuts casing running time by as much as one third. Ask for Catalog Supplement No. 325.

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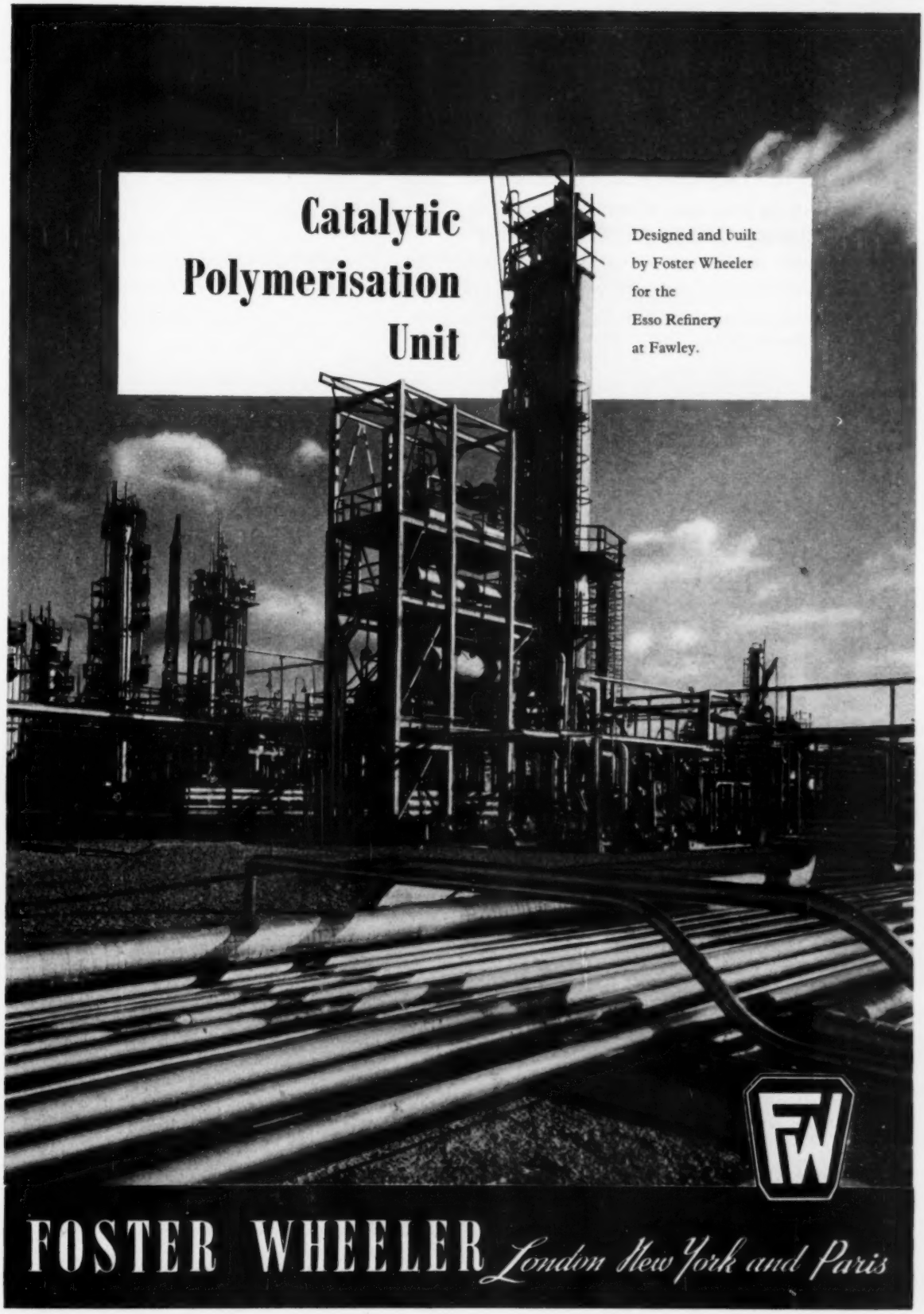
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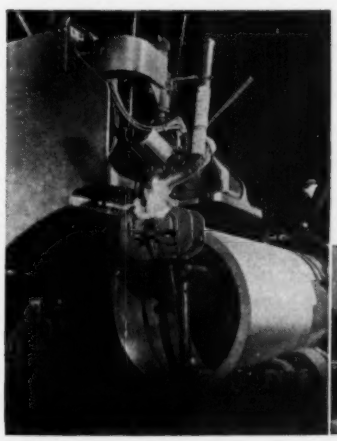
Bottom Right
A Babcock fusion-welded treating tower prior to despatch from the Company's Renfrew Works.

Below
Automatic fusion-welding of a thick-walled pressure vessel at Renfrew Works.



The 75 ft.-long by 10 ft.-diameter pressure vessel shown above during installation at the Patchway Works of Bristol Aero-Engines Limited, is part of a special test cell nearly 90 ft. long fabricated by Babcock & Wilcox Ltd. in molybdenum steel, by the *BABCOCK fusion-welding process.*

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